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Production of 1,3-Butadiene from Propylene

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Abstract

Our proposed plant design produces 103 million lb/year of 1,3 butadiene from propylene. Today, there are three chief methods to produce 1,3 butadiene. These include the Houdry process, oxidative dehydrogenation of 2-butenes and steam cracking of saturated hydrocarbons. The latter is the most widely used. The primary motivation behind this project was the production of 1,3 butadiene without the need for olefin cracker C4 crude oil streams. Olefin cracker C4 streams will decrease in availability as the trend towards lighter feedstock increases. Our plant is divided into four sections, namely metathesis, distillation, oxidative dehydrogenation and extractive distillation. The two byproducts include gasoline and ethylene. 1,3 butadiene is separated through extractive distillation with the help of solvent, NMP and is 99.9533% pure. The cost of purchase of propylene is $0.65/lb and the selling cost of 1,3 butadiene is $1/lb. However, it costs 2 propylene molecules to make one molecule of butadiene. This report provides a detailed design and economic analysis for 1,3-butadiene production in the Gulf Coast. Process flow sheets, energy and utility requirements and reactor design have been considered during our analysis below. The total cost of equipment is $44,918,915 and the variable cost is $200,958,000. Due to the large amounts of propylene, NMP and utilities required, our process is not profitable. The exploration of the metathesis step catalyst to improve 2-butene yields would significantly help the process. Profitability is also heavily dependent to the price ratio of 1,3 butadiene to propylene. We expect based on our market research that the cost of 1,3 butadiene will rise in the future.

Disciplines

Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

UNIVERSITY OF PENNSYLVANIA, DEPARTMENT OF CHEMICAL AND BIOMOLECULAR ENGINEERING

Production of 1,3-Butadiene from Propylene

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4/14/2015

University of Pennsylvania
School of Engineering & Applied Science
220 S 33rd Street Philadelphia, PA 19104
April 15, 2015

Dear Mr. Fabiano and Dr. Riggleman,

Enclosed is our proposed project design to convert propylene to 1,3-butadiene in response to the project suggested by Mr. Gary Sawyer. This process addresses a growing need for 1,3-butadiene. The demand for 1,3-butadiene will rise as lighter feedstocks such as ethylene prove to be more lucrative. As the demand for lighter feedstock increases, the availability of C4 crude oil and therefore 1,3 butadiene decreases. Therefore, this proposed method does not use C4s as a starting raw material for 1,3-butadiene production.

Our process is made up of four main parts: metathesis, distillation, oxidative dehydrogenation, and extractive distillation. Our aim was to produce 100 million lb of 1,3-butadiene/ year. Therefore, a feed of 258,000,000 lb propylene /year is being consumed by our plant. The two byproducts that emerge from this process and are sold for a profit are ethylene and gasoline. The solvent for extractive distillation, NMP is recycled and only 1% of the total extractant needed has to be replaced annually.

This report focuses on the overall process design and economic analysis of the 1,3-butadiene plant. It provides detailed process flowsheets, equipment and utility costs, and reactor design. A major hurdle is in the metathesis process, where a 15% conversion per pass of propylene is expected. Extensive research has to develop a suitable metathesis catalyst to improve metathesis before this project can be implemented.

Thank you for your assistance,

Safia Haidermota	Amanda Nestlerode	Victor Ngo

CBE 459 Senior Design Project:

SYNTHESIS OF 1,3 BUTADIENE FROM PROPENE

By:
Safia Haidermota, Amanda Nestlerode, and Victor Ngo

Presented To:
Mr. Leonard Fabiano, Dr. Warren Seider, Dr. Riggleman, and Mr. Sawyer

April 11, 2015
Department of Chemical and Biomolecular Engineering
University of Pennsylvania
School of Engineering and Applied Science

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1.0 ABSTRACT

Our proposed plant design produces 103 million lb/year of 1,3 butadiene from propylene. Today, there are three chief methods to produce 1,3 butadiene. These include the Houdry process, oxidative dehydrogenation of 2-butenes and steam cracking of saturated hydrocarbons. The latter is the most widely used. The primary motivation behind this project was the production of 1,3 butadiene without the need for olefin cracker C4 crude oil streams. Olefin cracker C4 streams will decrease in availability as the trend towards lighter feedstock increases.

Our plant is divided into four sections, namely metathesis, distillation, oxidative dehydrogenation and extractive distillation. The two byproducts include gasoline and ethylene. 1,3 butadiene is separated through extractive distillation with the help of solvent, NMP and is 99.9533% pure. The cost of purchase of propylene is $0.65/lb and the selling cost of 1,3 butadiene is $1/lb. However, it costs 2 propylene molecules to make one molecule of butadiene.

This report provides a detailed design and economic analysis for 1,3-butadiene production in the Gulf Coast. Process flow sheets, energy and utility requirements and reactor design have been considered during our analysis below. The total cost of equipment is $44,918,915 and the variable cost is $200,958,000. Due to the large amounts of propylene, NMP and utilities required, our process is not profitable. The exploration of the metathesis step catalyst to improve 2-butene yields would significantly help the process. Profitability is also heavily dependent to the price ratio of 1,3 butadiene to propylene. We expect based on our market research that the cost of 1,3 butadiene will rise in the future.

2.0 INTRODUCTION

1,3-butadiene is a primarily used as a chemical intermediate and as a monomer in the manufacture of polymers. Chemical intermediates manufactured from butadiene include adiponitrile and chloroprene. Adiponitrile is used to make nylon fibers while chloropene makes a variety of products such as wet suits, gaskets and hoses. Polymers made from butadiene include synthetic rubbers such as styrene-butadiene rubber (SBR) and polybutadiene rubber (PBR) and nitrile rubber. Butadiene is also used in the commercial production of butanediol and tetrahydrofuran. Butanediol is the feedstock for polymer resins while tetrahydrofuran is vital for the production of spandex fibers (American Chemistry Council, 2015).

Currently, 1,3 butadiene is produced primarily via the steam cracking of saturated hydrocarbons. Butadiene is then extracted from olefin cracker crude C4 streams. 1,3 butadiene has two other commercial methods of production known as the Houdry Process and Oxydehyrogenation. The Houdry process involves the dehydrogenation of butane gas to form 1,3 butadiene, while oxydehydrogenation converts 2-butenes to 1,3-butadiene. All three processes require readily available C4 molecules. However, there is an increased trend towards lighter feedstock and the C4 molecule will soon be in short supply.

The focus of this report is to make 1,3 butadiene via propylene to match the demand. The first step involves a process known as metathesis. Metathesis reacts two propylene molecules to make ethylene and 2-butene. Other compounds that are produced as a result of side reactions are 1-butene, pentenes and hexenes. However, to make this process selective and only produce ethylene and 2-butene, a suitable catalyst is required. There is no such catalyst in operation today. However, from 1966-1972, Phillips Petroleum ran this method using $W0_3/SiO_2$ as a catalyst. However, in the last 40 year, there has been a great deal of advancement in catalyst development techniques, therefore a new catalyst needs to be explored. Ethylene and gasoline are distilled and separated and then sold as byproducts. Once 2-butene is produced, it is converted to 1,3 butadiene via oxidative dehydrogenation via the below reaction.

$$C_4H \text{ (2-butene)} + 0.5\ O_2 \rightarrow C_4H_6 \text{ (1,3-butadiene)} + H_2O$$

Once 1,3 butadiene is produced, it needs to be separated out via extractive distillation. N-methylpyrrolidone (NMP) is used as a solvent. 1,3 butadiene needs to be separated from water, non condensables, cis and trans butenes and NMP. The purity of 1,3 butadiene required is 99.5%

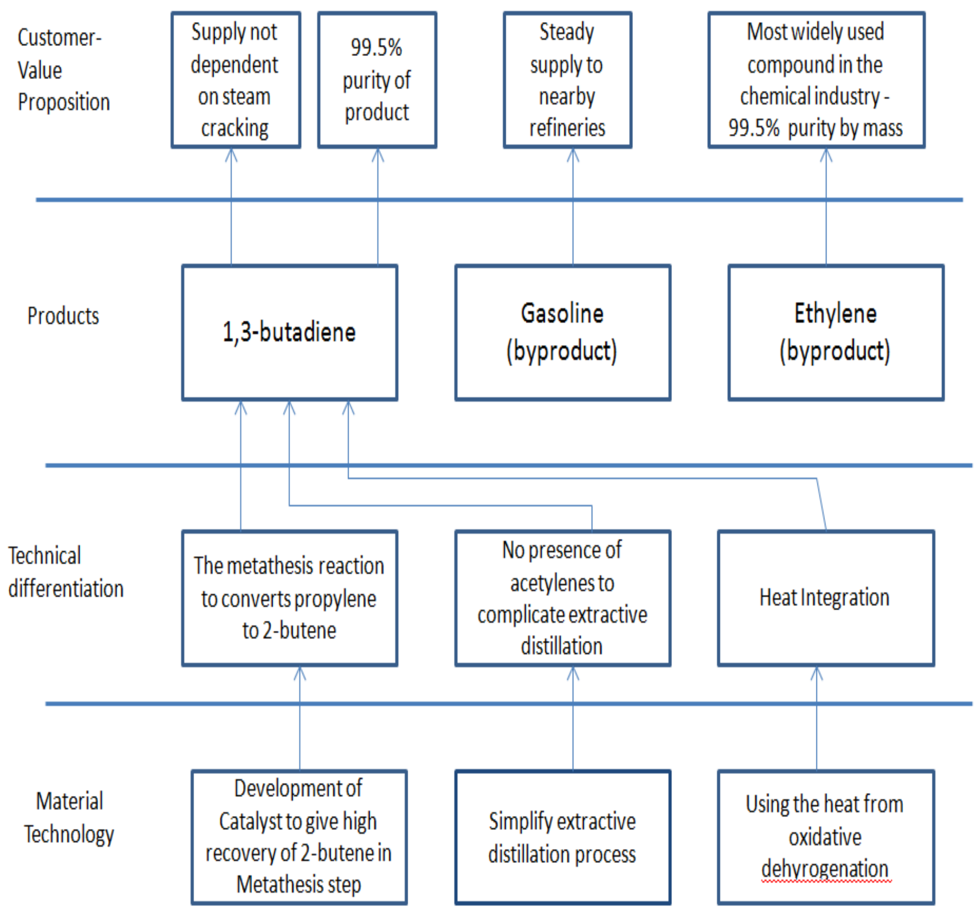
and it is achieved. In the report below, multiple factors such as utility requirements, plant design and equipment costs are considered and discussed.

3.0 OBJECTIVE TIME CHART

Name:	Production of 1,3 Butadiene from Propylene
Champions	Mr. Leonard Fabiano, Dr. Rob Riggleman, and Mr. Gary Sawyer
Project Leaders:	Amanda Nestlerode, Safia Haidermota, and Victor Ngo
Specific Goals:	Development of a process to convert propylene to 1,3-butadiene
Project Scope:	*In Scope*
	Annual production of 100 million lb of 1,3- butadiene
	1,3-butadiene purity of 99.5% (by mass)
	Economic Analysis
	Plant Design and Size
	Reactor Design and Specifications
	Out of Scope
	Lab work to design and test catalyst for metathesis process
	Experimental procedures
Deliverables:	Mass and energy balances of the process
	Equipment specifications, designs, and cost estimates
	Detailed flow sheet diagrams and simulation results
	Economic and profitability analysis, with an emphasis on overall feasibility
	Reactor Design and Analysis
Time Line:	Completed this design project within three months

4.0 TECHNOLOGY READINESS ASSESMENT

4.1 INNOVATION MAP



4.2 Market and Competitive Analysis

1,3-butadiene is primarily used as a chemical intermediate and as a monomer in the manufacture of polymers. More than 75% of butadiene product goes into synthetic rubbers. The single largest use of 1,3 buatdiene is in the form of PBR to make automobile tires (35%), followed by polybutadiene rubber (22%), adipronitrile (13%) and neoprene rubber (5%). Other major products include latex, gaskets, hoses, seals, nylons, pipes and paints.

Butadiene is currently prepared by the thermal cracking of saturated hydrocarbons, with naptha being used as a raw material. This accounts for 91% of the world's butadiene supply (Product Stewardship Manual, 2010). In the United States, the availability of crude C4 has become a significant factor in the market due to the increased demand for ethylene. Ethylene is one of the most important chemicals in American manufacturing and is a building block for numerous chemicals that range from plastic to antifreeze solutions and solvents. Naptha is also the main raw material for ethylene, therefore a direct competition for raw materials occurs. In the past, like in January 2013, there were two planned ethylene cracker outages on the USGC that caused the crude C4 supply to tighten up. Demand for ethylene feed in the third quarter of 2013 was 3.6% higher than the production in the fourth quarter of 2012. In an article released by ICIS in 2014, new projects mat raise US ethylene capacity by 52% and polyethylene production by 47% (Chang 2014).

Another reason for the possible future shortage of butadiene is the shale gas boom in the US. The percentage of C4 hydocarbons required for the production of butadiene is very low in natural gases compared to naptha or crude oil. Last year, the US butadiene demand was 1.9 million tons and the US produced 1.6 million. GBI research predicts that the demand for butadiene will hit 2.4 million tons by 2020 and result in an import of 524,916 tons by 2020.

Propylene, which is our raw material, can be made from propane, which is relatively cheap and plentiful. The long-term outlooks of the gas and propane markets appear to favor propylene. Dow Chemical plans to build a world-scale propylene dehydrogenation (PDH) plant in Freeport, Texas by 2015, and the company aspires to build another plant by 2018. The PDH process takes propane as feedstock and converts it into high-purity propylene. Currently, only Houston-based PetroLogistics uses the process to make propylene, and the company plans to expand in the near future. LyondellBasell, meanwhile, plans to build a unit in Texas with the hope that it would increase propylene production by roughly 500 million pounds. All the above data indicates that there needs to be an alternate form to produce butadiene on a large scale.

4.3 Preliminary Process Synthesis

As mentioned in the market and customer requirements, the primary motivation behind this project was the production of 1,3 butadiene without the need for olefin cracker C4 crude oil streams. Propylene was envisioned as a good starting point since it's production may increase via the dehydrogenation of propane. The metathesis reaction that converts propylene to 2-butene has not been carried out in industry today and a specialized catalyst needs to be specifically created.

Propylene can be converted to 2-butene and ethylene through the specialized metathesis reaction. The basic chemistry in a vapor phase, equilibrium-limited reaction, is:

$$C\text{-}C{=}C + C\text{-}C{=}C \rightarrow C\text{-}C{=}C\text{-}C + C{=}C$$

More generally, the reaction exchanges the double bonds as:

$$R1\text{-}C{=}C\text{-}R2 + R3\text{-}C{=}C\text{-}R4 \rightarrow R1\text{-}C{=}C\text{-}R3 + R2\text{-}C{=}C\text{-}R4$$

If the metathesis reaction is very selective, then the only products are 2-butene and ethylene. A catalyst to meet our specifications needs to be developed in the laboratory. Since this is not a reaction in current industrial practice, there is little reaction or catalyst information available. However, this process was developed at Phillips Petroleum in the 1960s. The Philips Triolefin Process used a heterogenous W03/Si02 catalyst to convert propylene to ethylene and 2-butene. This process ran from 1966-1972 but it was shut down due to the increased demand for polyproylene. Today, Lummus Technology's patented Olefin Conversion produces 4 million tons of propylene from C4 feedstock. Metathesis reactions are in general, energy neutral, which translates into low plant energy cost. Therefore, they make sense economically to pursue. Other insights from the Lummus Techonology process include that a small amount of coke is formed on the catalyst, so the beds are periodically regenerated with nitrogen-diluted air. The duration of the regeneration depends on the specific catalyst designed but a starting estimate is 3 weeks. This reaction is further explained in the upcoming section on Reactor Design.

Finally, Oxidative Dehydrogenation and Extractive Distillation are both common commercial practices and patents were referenced to model these processes. This report focuses on optimizing a single design with required specifications of the problem statement located in Appendix A.

4.4 Assembly of Database

Economic and process design decisions were carefully made based on information in the problem statement, market reports and faculty and consultants expertise.

The economic analysis for this report is based on the parameters and guidelines indicated in the problem statement. The price of 1,3 butadiene and propylene were $1/lb and $0.65/lb respectively. Through our research, the price of NMP was set at $1.50/lb. A small portion of relatively pure NMP is purged during extractive distillation and is sold for $1.25/lb. Other by products such as ethylene and gasoline are sold at $0.60/ lb and $0.12/lb respectively. Our target butadiene production was specified as 100 million lb/year, therefore the propylene feed had to be adjusted to meet that mark. Aspen Process Economic Analyzer (APEA) provided equipment costing for all equipment except reactors and storage tanks. Costing spreadsheets were used for reactors and storage tanks.

The process design was simulated in Aspen Plus. In order to model the thermodynamic and physical interactions of our materials, the RK SOAVE property method was specified for Metathesis, Distillation and Oxidative Dehydrogenation. NRTL property method was used to model the extractive distillation. An important point is that Aspen Plus was asked to estimate interactions between the molecules; therefore there may be some discrepancies especially when modeling extractive distillation.

The problem statement specified conditions for the metathesis reaction since that reaction is not commercially available. The temperature conditions and pressure were 150 C and 2 atm respectively. The optimum conditions for this reaction will be explored in the Reactor Design section. In order to size the reactor, the space velocity of 20 kg feed/catalyst/hour was specified. The propylene conversion per pass was 15% at equilibrium. For the oxidative dehydrogenation reaction, the temperature conditions and pressure were 150 C and 2 atm respectively. In order to size the reactor, the space velocity of 1.5 kg feed/catalyst/hour was specified. According to the problem statement, the butene conversion per pass was 95% at equilibrium and the butene selectivity for butadiene is 95%.

5.0 PROCESS FLOW DIAGRAMS AND MATERIAL BALANCES

This process is divided into four sections as stated below:

Section 100: Metathesis

Section 200: Distillation

Section 300: Oxidative Dehydrogenation

Section 400: Extractive Distillation

Each section is explained in the following pages using stream tables and process diagrams. A basic schematic of our process is presented below.

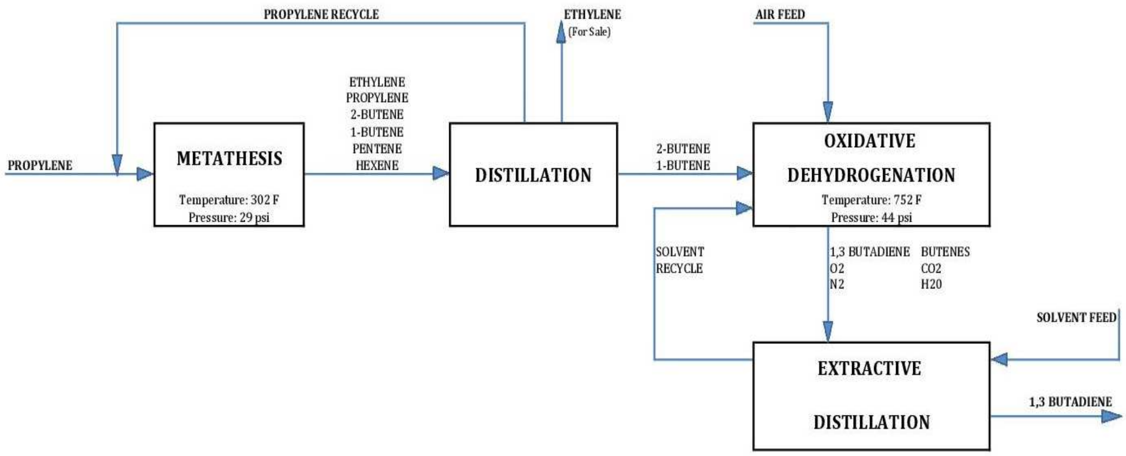


Figure 5.1.1: Depiction of Overall process

5.1 OVERVIEW

The process of converting propylene to butadiene is composed of five different sections which describe in detail the production of 100 million lbs/yr of 1,3-butadiene from propylene. First, the propylene feed undergoes metathesis [Section 1] to produce cis-2-butene, trans-2-butene, ethylene, pentene, and hexene. This metathesis also considers the isomerization of 2-butene to 1-butene. Excess propylene is recycled and the remaining products are fed into the next step. Following this metathesis reaction is a series of distillations [Section 2] to separate butenes in preparation for the oxidative dehydrogenation [Section 3]. A reactor is fed with the effluent butene from distillation and fresh air (21% O_2, 79% N_2 by mass). This reactor converts the butenes into 1,3-butadiene, the final product of the process. The dehydrogenation also contains combustion reactions. The products carbon dioxide, oxygen, nitrogen, and water along with the butadiene and butenes are sent into a column where the non-condensable vapors are vented. The final step in the process is extractive distillation [Section 5] using n-methyl-2-pyrrolidone as the solvent to remove 1,3-butadiene from the remaining C4's.

5.2 SECTION 100: METATHESIS OF PROPYLENE TO 2-BUTENE

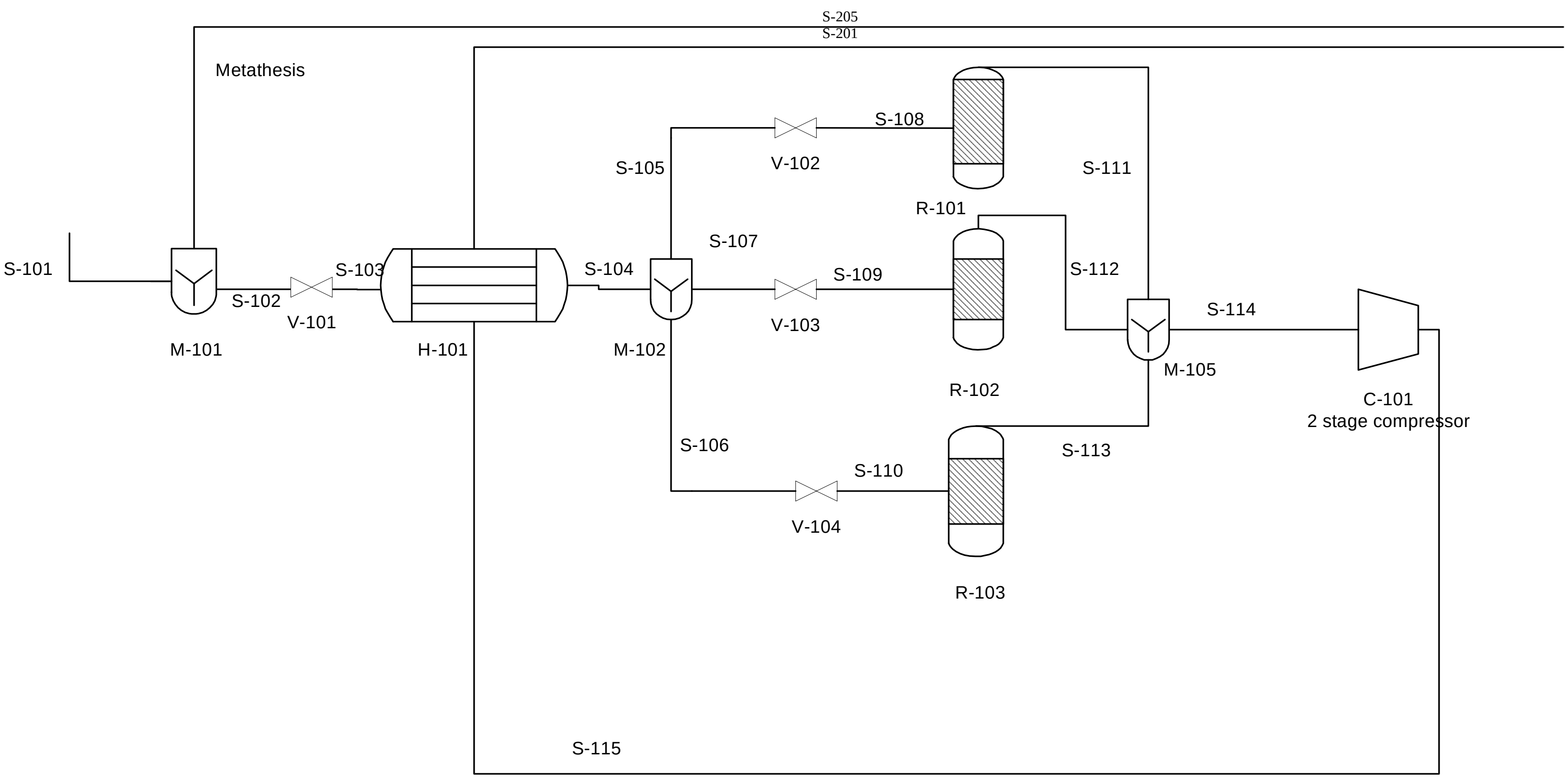


Figure 5.2.1: Diagram of Metathesis Process

Table 5.2.1: Mass Balance describing Section 100: Metathesis

METATHESIS				
COMPONENT Flow (lb/hr)	Inlet		Outlet	Difference
	S-101	S-205	S-201	
PROPYLENE	33665	52643	53373	**32935**
ETHYLENE		84	11653	**-11569**
TRAN-BUT		10022	20135	**-10113**
CIS-BUT		5242	12372	**-7130**
1-BUTENE		2423	3674	**-1251**
CIS-C6			23	**-23**
TRANS-C6			95	**-95**
CIS-C5		24	732	**-708**
TRANS-C5		72	2118	**-2046**
TOTAL MASS FLOW (lb/hr)	33665	70510	104175	**0**

The metathesis of propylene to 2-butene is covered in this first section. The feed into the process is sent into a reactor to perform the conversion and to form products cis-2-butene, trans-2-butene and the byproducts 1-butene, pentene, and hexene. The process is divided into three identical reactors in parallel to accommodate smaller vessel sizes. The specifications for each are the same, and this allows for the simultaneous operation of two reactors, while the remaining third reactor can decoke and be cleansed. This prevents lost days of operation due to any necessary maintenance in this section.

The feed stream of pure propylene, S-101, is supplied to the first section of the process at 77 F and 29 psi. Propylene is commercially available as a liquid at 350 psig and ambient temperature with purity of 99.5% (the balance propane). The required molar flow rate for 100 million lb/yr of butadiene production is 520 lbmol/hr of propylene provided by the problem statement specifications. This was calculated based off of the specified propylene conversion per pass of 15% in the metathesis reaction, carbon selectivities of 32% ethylene, 63% butene, and 44% pentene and hexene in the metathesis, and finally a butene selectivity to butadiene of 95%. However, during simulation, other factors such as efficiency, recovery, and purity were non-ideal, so the feed was adjusted to 800 lbmol/hr to produce 100 million lbs/yr of butadiene. This excess provided a production rate of butadiene

S-101 is mixed with the propylene recycle stream from the effluent of a distillation column to be discussed later in section 2. The mixed stream, S-102, is then pressure reduced to

29 psi, exiting P-101 as stream S-103, and then heated using heat from the metathesis effluent in heat exchanger H-101 to 302 F. The modified feed, S-104, splits into three identical streams and is fed into the parallel reactor vessels.

In reactors R-101, R-102 and R-103, the conditions for the metathesis reaction are a pressure of 2 atm and 150 C, or 29 psi and 302 F. This reaction consists of converting propylene into cis and trans-2-butene given the following vapor phase equilibrium reaction:

$$2C_3H_6 \rightarrow C_4H_8 + C_2H_4 \quad (1)$$

Propylene is typically made by steam cracking olefin feedstocks. The natural gas boom in recent years in the United States due to hydraulic fracturing in the Marcellus Shale, Eagle Ford Shale, and the Bakken Shale all attribute to a lighter feedstock for steam cracking. The facilitation of propylene production also improves the efficiency of forming butadiene. With this metathesis reaction the production of C4 is more readily available, and the production of butadiene from oxidative dehydrogenation, a well known process, can be done with the C4 as a feed.

The flowrate of the metathesis feeds are 52,130 lbs/hr, with a propylene mass fraction of 0.83. In Aspen, reaction (1) was modeled using REQUIL in block MET1. This block reacted the propylene in stream S-104 to cis-2-butene and trans-2-butene using a temperature approach specification of 0 F.

Catalyst Description:

The main objective of the project is to analyze the profitability of the production of butadiene from propylene given the metathesis reaction to first convert propylene to butene. This requires a selective catalyst to improve the conversion as well as the kinetics. Information on the metathesis of propylene to butene is very sparse. However, if the catalyst for reaction is very selective, then the only products are the cis- and trans-2-butenes. Unfortunately, metathesis to produce propylene from butene is more known than the reaction of interest here, reaction (1). The propylene conversion to butene, in fact, was practiced in the early 1970's, but was discontinued and information regarding ideal catalysts are not readily available. Therefore, a catalyst that is selected will most likely be non-ideal. This would lead to side reactions including the isomerization of 2-butene to 1-butene given below:

$$\text{2-Butene} \rightarrow \text{1-Butene} \quad (2)$$

The isomerization of 2-butene to 1-butene was modeled using units R-102 and R-105, RSTOIC blocks in Aspen. Preliminary analysis set the fractional conversion of both cis and trans-2-butene to 10% and was followed by a sensitivity analysis up to 100% conversion. Finally, 4 possible side reactions were modeled in units R-103 and R-106, another set of REQUIL blocks, specifying the the following reactions:

$$2\ \text{1-Butene} \rightarrow C_2H_4 + C_6H_{12}\ (3)$$

$$C_3H_6 + \text{1-Butene} \rightarrow C_2H_4 + C_5H_{10}\ (4)$$

where pentene and hexene cover both cis and trans. The effluents of the reactors are combined into a single stream, S-113, and leaves at a temperature of 302 F and a pressure of 29 psi. Before distillation, the stream has to be compressed and cooled.

5.3 SECTION 200: DISTILLATION TO RECOVER BUTENES

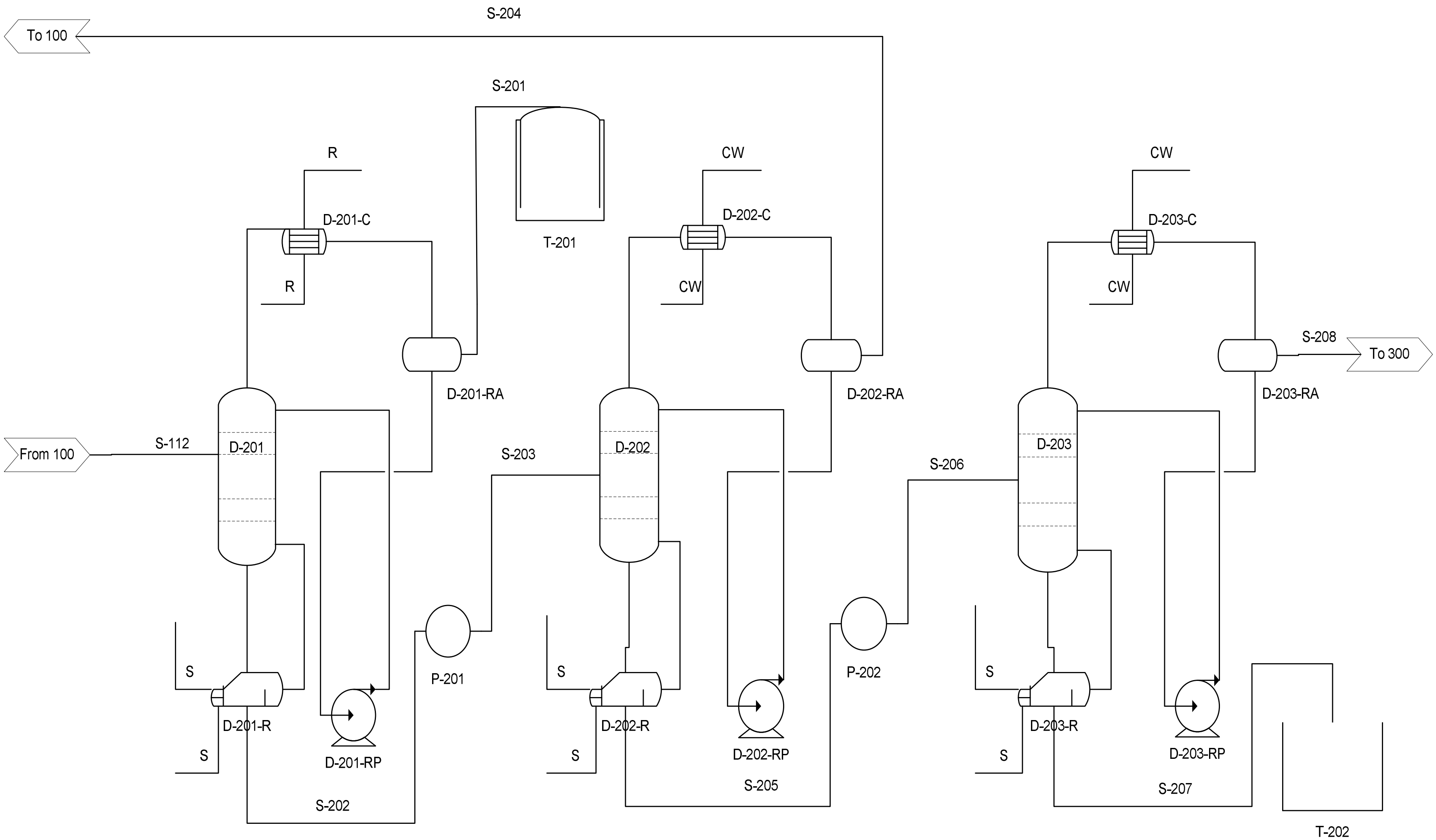


Figure 5.3.1: Diagram of the Distillation Process

Table 5.3.1: Mass Balance describing Section 200: Distillation

DISTILLATION						
COMPONENT Flow (lb/hr)	**Inlet**	**Outlets**				**Difference**
	S-112	**S-201**	**S-204**	**S-207**	**S-208**	
PROPYLENE	53312	175	52606	531		**0**
ETHYLENE	11593	11581	12			**0**
TRAN-BUT	20234		10132	10017	85	**0**
CIS-BUT	12433		5305	7033	95	**0**
1-BUTENE	3691		2443	1244	4	**0**
CIS-C6	23				23	**0**
TRANS-C6	96			1	95	**0**
CIS-C5	739		24	213	502	**0**
TRANS-C5	2137		73	648	1416	**0**
TOTAL MASS FLOW (lb/hr)	**104258**	**11756**	**70595**	**19687**	**2220**	**0**

The second step of the process is to recover the butenes that were produced in the metathesis reactions. This is done using three distillation columns with pumps in between each column to make up for losses in pressure. Ethylene will be separated and sold off at an industry specified purity of at least 99.5% in the distillate of the first distillation column. In the second column, propylene will be recovered in the distillate and recycled back into the metathesis feed. Finally, the butene products will be separated from the side products, C5 and C6, in order to undergo the oxidative dehydrogenation in section 3.

The effluent of the metathesis, stream S-120, is first compressed from its vapor state in block C-101 to the required pressure of the first column, 400 psia, with a resulting compressed temperature of 574 F. The stream is then cooled to 160 F before entering the first column in H-101 with the metathesis feed as the coolant. Here, the Aspen flow sheet shows two heat exchangers, H-101 and H-102, but each represents one side of a single counter current shell and tube heat exchanger where the cold side is the metathesis feed and the hot side is the effluent of the metathesis coming out of the compressor. This was a result of Aspen being unable to converge the mass balance with the two recycle loops.

The first distillation column, the radfrac block, D-201, uses two distillate design specifications. The first specified the recovery of ethylene in the distillate to be 99% and the second stipulated a purity of ethylene in the distillate of 99%. The parameters that were varied to achieve these specifications were the distillate to feed ratio and reflux ratio. Stream S-112 enters the column on stage 10 and exists at 160 F and 400 psi. The results converged with the ethylene flow rate of 11800 lbs/hr at 2 F and 400 psi, where it would be sent into a storage tank before being sold. The bottoms containing the rest of the products were fed into pump P-201 to resolve pressure differences before entering column D-202.

Stream S-203 enters column D-202 at 182 F and 300 psi above stage 5. This distillation was used to separate to propylene from the remaining products in order to recycle the propylene back into metathesis. In this case, the purity of propylene is not a major concern since it won't be sold. The propylene is recycled to mix with stream S-101 at a temperature of 139 F and 300 psi, which is already similar enough statewise to perform a safe mix of streams.

The bottoms of column D-202 is pumped through to column D-203 at a temperature of 240 F and 103 psi and fed halfway up the column on stage 5. This third column was used to remove the sideproducts from the butenes, which will react to produce the final product, 1,3-butadiene, in the oxidative dehydrogenation reactor. The distillate of the column had a total butene flow rate of 18,300 lbs/hr, a 99% recovery. The bottoms containing pentene and hexene are sent into a storage tank in order to be sold off as gasoline products.

5.4 SECTION 300: OXIDATIVE DEHYDROGENATION

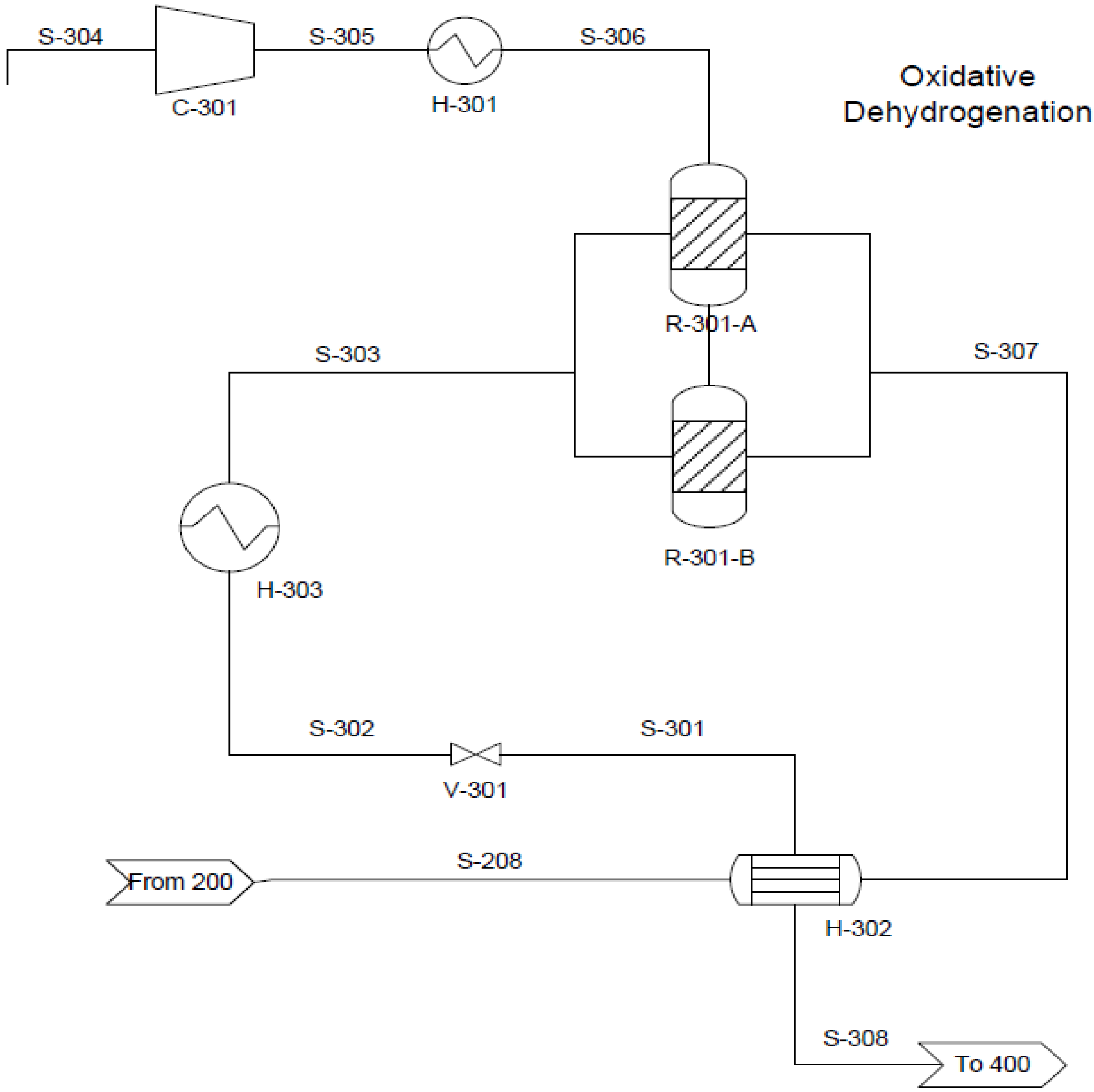


Figure 5.4.1: Diagram of the Oxidative Dehydrogenation Process

Table 5.4.1: Mass Balance Describing Section 300: Oxidative Dehydrogenation

OXIDATIVE DEHYDROGENATION				
COMPONENT Flow (lb/hr)	Inlets		Outlets	Difference
	S-208	S-306	S-307	
PROPYLEN	535		535	**0**
TRAN-BUT	10025			**10025**
CIS-BUT	7032			**7032**
1-BUTENE	1247		1247	**0**
1:3BUTADIENE			15622	**-15622**
CARBON DIOXIDE			2676	**-2676**
OXYGEN		7566	27	**7539**
NITROGEN		24919	24919	**0**
H20			6298	**-6298**
TRANS-C6	1		1	**0**
CIS-C5	208		208	**0**
TRANS-C5	633		633	**0**
TOTAL MASS FLOW (lb/hr)	19681	32485	52166	**0**

The purified butene mixture leaves as the distillate from column D-203 in stream S-208. At this point, the stream has been condensed and cooled to a liquid at 143 °F and 100 psia, and must be heated and vaporized prior to entrance to the oxidative dehydrogenation reactor, which runs at 752 °F and 44 psia. To meet this requirement, the stream is heated in a shell-and-tube heat exchanger, H-301, using the hot outlet stream from the reactor (stream S-306) as the hot fluid and stream S-208 as the cool fluid. This heats the stream to 449.2 °F, which requires further heating before it may be fed to the reactor. Pressure is relieved from the stream using a valve, V-301, which reduces the pressure from 100 psia to the reactor operating pressure of 44 psia. The stream is then heated to its final temperature of 752 °F in a shell-and-tube heat exchanger, H-303, using steam as the hot fluid. At this point, the reactor feed is at the necessary temperature and pressure, 752 °F and 44 psia, and is fed into the shell-and-tube, packed bed reactor (R-301).

Air must also be fed into the reactor, and was chosen over pure oxygen or oxygen-enriched air based on patent specifications in order to reduce unwanted combustion side reactions and also because the large volume of inert nitrogen aids in absorbing the large amount of heat produced during this reaction to prevent the vessel from overheating. Air must first be pressurized and then heated from room temperature and atmospheric pressure (68 °F and 15 psia) to the reactor feed conditions of 752 °F and 44 psia. In order to do this, a gas compressor is used followed by a shell-and-tube heat exchanger using steam as the hot fluid. The feed rate of air was selected based on patent specifications calling for an optimal oxygen:n-butene ratio of from 0.55 to 10. To reduce the necessary vessel size and costs, the amount of air was optimized down to the minimum requirement of 0.5% excess oxygen, giving an oxygen:n-butene ratio of 0.778, which is within the optimal range.

The oxidative dehydrogenation reaction is carried out in a fixed-bed shell-and-tube packed bed reactor operating at 752 °F and 44 psia. The reactor is carried out in a single shell, though a second shell is purchased for the purpose of catalyst regeneration and maintenance. The reaction uses a multimetal oxide catalyst to achieve optimal conversion. In this case, the chosen catalyst has the formula $Mo_{12}BiFe_{0.1}Ni_8ZrCr_3K_{0.2}O_{53}$, and the reaction that occurs is highly exothermic with four primary reactions occurring simultaneously. Fraction conversion is given on a molar basis using either cis- or trans- butene as the referene component.

Table 5.4.2: Reaction Specifications for the Oxidative Dehydrogenation Process

Reaction	**Conversion**	**Heat of Reaction (Btu/lbmol)**
C_4H_8-2 (cis) + 0.5 O_2 → C_4H_6-4 + H_2O	95%	-53,881
C_4H_8-3 (trans) + 0.5 O_2 → C_4H_6-4 + H_2O	95%	-52,333.5
C_4H_8-2 (cis) + 6 O_2 → 4 CO_2 + 4 H_2O	5%	-1,089,600
C_4H_8-3 (trans) + 6 O_2 → 4 CO_2 + 4 H_2O	5%	-1,088,050

The combustion reaction in which either cis- or trans-2-butene reacts with oxygen to form carbon dioxide and water is an undesired side reaction, and while the catalyst yields greater selectivity for the primary reaction in which 1,3-butadiene is produced, it cannot entirely eliminate the side reactions. The reactor conditions of 752 °F and 44 psia were selected in order to give this optimal selectivity for 1,3-butadiene production. The oxidative dehydrogenation reaction is maintained at the isothermal operating condition of 752 °F by using a cooling fluid in the shell-side of the reactor. Potassium nitrate was chosen as the liquid heat transfer media due to its ability to handle high heats up to 914 °F.

The reactor effluent leaves at 752 °F and 44 psia, and must be cooled before being purified in the extractive distillation. To reduce utility costs, the stream is used as the hot fluid in the countercurrent shell-and-tube heat exchanger (H-302) also used to heat up the reactor inlet feed. This cools the reactor effluent to 485.3 °F and raises the pressure to 300 psia. At this point, the reactor effluent is fed to the extractive distillation part of the process.

5.5 SECTION 400: EXTRACTIVE DISTILLATION

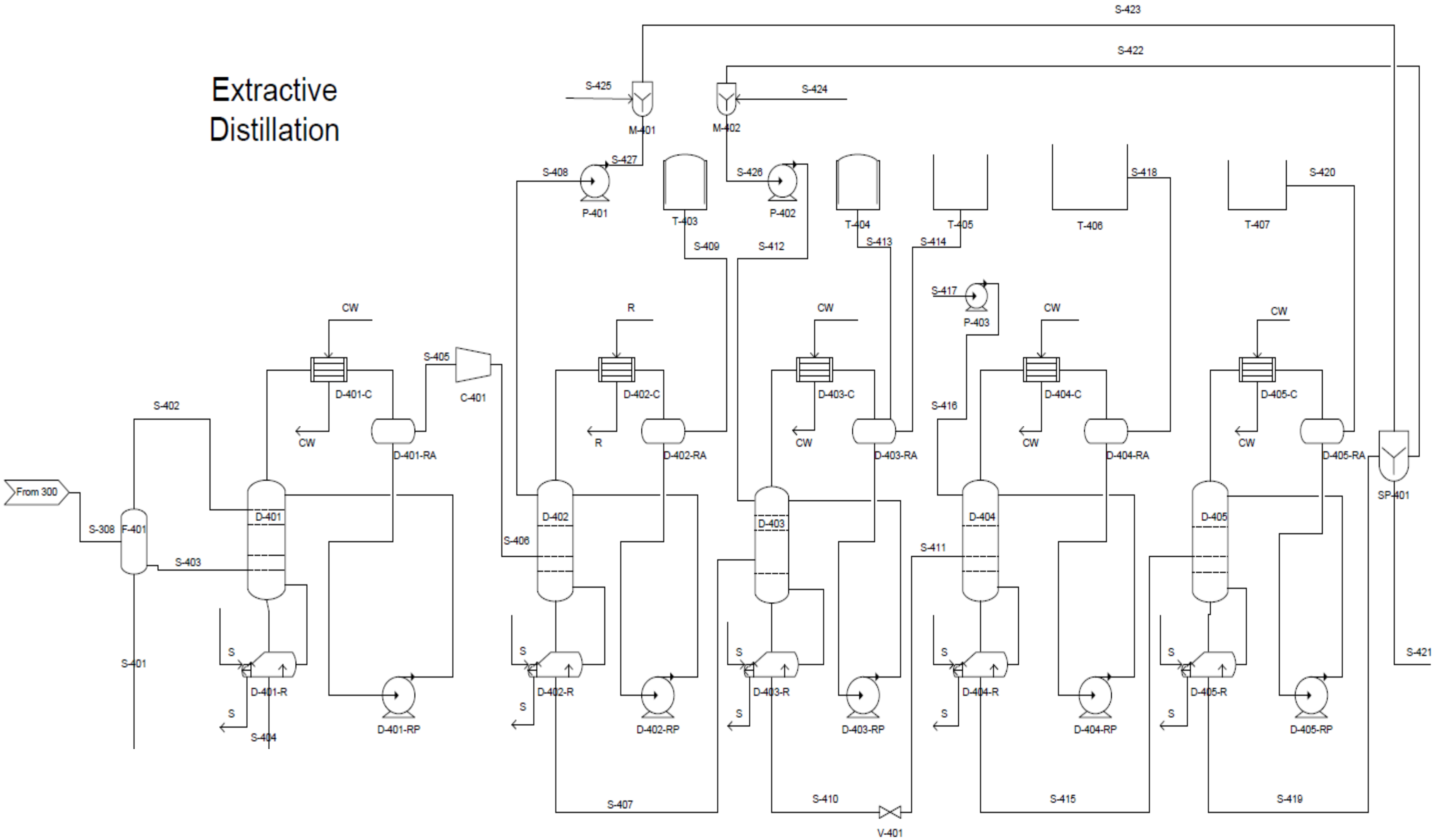


TABLE 5.5.1: MASS BALANCE DESCRIBING SECTION 400: EXTRACTIVE DISTILLATIO

EXTRACTIVE DISTILLATION										
COMPONENT Flow (lb/hr)	**Inlets**		**Outlets**							**Difference**
	S-308	**S-418**	**S-405**	**S-407**	**S-409**	**S-410**	**PRODUCT**	**S-415**	**PURGE**	
PROPYLEN	535		0	375	106	16	39	0	0	**-1**
1-BUTENE	1247		0	0	2	1	57	1187	0	**0**
1:3BUTADIENE	15622		0	330	912	383	13038	959	0	**0**
CARBON DIOXIDE	2676		0	2539	132	4	0	0	0	**1**
OXYGEN	27		0	27	0	0	0	0	0	**0**
NITROGEN	24919		0	24660	258	1	0	0	0	**0**
H20	6298		6287	0	0	0	0	11	0	**0**
TRANS-C6	1		1	0	0	0	0	0	0	**0**
CIS-C5	208		4	0	0	0	0	204	0	**0**
TRANS-C5	633		10	0	0	0	0	623	0	**0**
NMP	0	1827	0	0	0	28	14	418	1367	**0**
TOTAL MOL FLOW (lb/hr)	52166	1827	6302	27931	1410	433	13148	3402	1367	**0**

5.5 Section 400: Extractive Distillation

The reactor effluent from the oxidative dehydrogenation reaction contains a large amount of side products as well as inert nitrogen that was initially used for heat distribution in the highly exothermal reaction. As a result, stream S-308 entering extractive distillation is only about 30% butadiene by mass, and 48% nitrogen. There is also a significant amount of water, carbon dioxide, and 1-butene that must be removed in order to purify the 1,3-butadiene. The high-purity 1,3-butadiene that this system will be producing requires a purity of 99.5% by mass of butadiene. In order to achieve this high purity, an extractive distillation train will be used to recover the butadiene.

Before the extractive distillation, however, the reactor effluent (stream S-308) must be cooled and depressurized. All water in the system must also be removed, as the extractive solvent is intended to interact primarily with hydrocarbons and the presence of highly polar compounds such as water can negatively interfere with this process. Therefore, the impure butadiene stream is first fed into a flash vessel, which flashes to a temperature of 100 °F and a pressure of 105 psia. The flash vessel uses cooling water to do this. This temperature drop results in a partial condensation of the feed, and product leaves the flash vessel in separate liquid (S-403) and vapor (S-402) streams, both at a temperature of 100 °F and a pressure of 105 psia. The purpose of this vessel is for altering temperature and pressure, and not to achieve any degree of separation. The 1,3-butadiene splits 99.6% to the vapor stream and 0.4% to the liquid stream, and so both streams are recovered and fed to the water separation column (D-401).

The water separation column is designed to remove 99.8% of all water by mass, and at very high purity (99.8% by weight) so that disposal of waste water will not be an issue. The reflux ratio and number of stages were modified in order to determine the most cost-effective option, and 10 stages at a reflux ratio of 5 were selected. The pure water stream leaves the column in the bottoms at a temperature of 331 °F and a pressure of 104 psia, which may be given minimal treatment. The distillate leaves as a vapor, as it is composed largely of nitrogen (54.3% by weight) and therefore would require very low temperatures to condense. The vapor distillate leaves the column at 58 °F and a pressure of 101 psia. Before it can be fed to the first extractive distillation column, this stream must be compressed. A multi-stage isentropic compressor (C-401) uses two stages with an intermediate cooler to compress the stream to a pressure of 501 psia, resulting in a temperature of 100 °F. This stream, which is now only 86.8% vapor and the difference in liquid, is then fed to the first extractive distillation column.

Extractive distillation is a well-known process often used for the separation of hydrocarbons with very similar volatilities, such as of 1,3-butadiene and butenes. The process works by using a solvent, which absorbs a single component with much higher affinity. In this case, the solvent chosen was n-methyl-2-pyrrolidone (NMP), which has an affinity for 1,3-butadiene and therefore aids in its separation.

It should be noted that the modeling software used, Aspen Plus V8.6, was lacking many of the binary parameters for NMP interactions with various hydrocarbons (primary missing interactions included NMP/1-butene and NMP/trans-2-butene). While several different solvents were attempted (notably dimethylformamide and furfural), all solvents lacked key binary parameters when modeled in Aspen. These binary parameters were unavailable in literature, and so Aspen was used to estimate the parameters with UNIFAC. However, even with the parameter estimates, the results of the Aspen simulation deviated in certain behaviors from traditional extractive distillation patent specifications. This led to the conclusion that the Aspen-estimated parameters do not correctly model an extractive distillation process. The BASF patent on extractive distillation states that 1,3-butadiene is absorbed better by the solvent than butenes and therefore leaves in the bottoms of a distillation separating these two. However the Aspen simulation showed that 1,3-butadiene left columns in the distillate of column D-404, with the butenes flowing out of the bottoms. This deviation from patented extractive distillation information is notable, however as it results from a software error little could be done to correct for it, and thus the extractive distillation process was modeled to completion with this taken into consideration.

NMP was used for the extractive solvent, as Aspen had the greatest number of binary parameters available for NMP interactions. Although NMP has the drawback of being toxic, it is the most commonly used solvent for the separation of 1,3-butadiene and is notable for yielding a very pure product as well as being less corrosive than other solvents so that less expensive, steel construction can be used for all towers.

Four distillation columns are used in the extractive distillation, with the primary objectives of resulting in a high recovery and purity of 99.5% by weight of 1,3-butadiene, and of recovering most of the NMP for recycle. To reduce the cost of utilities, cooling water was used to meet most condenser cooling requirements, and steam was used to meet heating specifications unless otherwise noted. All columns were optimized by altering the reflux ratio and total number of stages to minimize both values. In two of the columns, high pressure (500 psia) was required to effectively separate components. The optimal feed rate of NMP was determined using design specifications in Aspen for each column.

In the first extractive distillation column, D-402, the compressed partial vapor stream composed primarily of nitrogen and 1,3-butadiene is fed to the bottom of the 15-stage column, while the extractive solvent, NMP, is fed to the top of the column as a liquid. The purpose of this column is to remove the non-condensable components (carbon dioxide, nitrogen, and oxygen) from the stream. This greatly reduces the volume of the stream, allowing the following columns to be smaller and thus decreasing costs. The distillate is entirely vapor, as in order to condense the distillate of primarily nitrogen it would have been necessary to cool to -270 °F, which required very large utility costs due to refrigeration and was not economical. To reduce this cooling requirement to the current value of -24 °F, the distillate was vented as a vapor and 2% of the butadiene was allowed into the distillate to raise the boiling point. The bottoms of the column contains 98% of the original butadiene and leaves as a liquid at 273 °F and 503 psia.

The remaining stream is primarily butadiene (23%) and NMP (73%) by weight. It is fed into stage 15 of the next, 20-stage, column (D-403), where additional NMP is also added to the top of the column. In this column, remaining amounts of propylene and non-condensable components are removed in the distillate of the column. The distillate stream is partial-liquid-vapor to minimize the heating requirements of the condenser, as small amounts of NMP, which has a normal boiling point of 400 °F, put a large heating stress on the condenser. These streams leave the column at 229 °F and 500 psia, and are collected into a storage tank to be sold as gasoline products. The bottoms of the column still contains the majority of the hydrocarbons with the NMP, and leaves the column at 426 °F and 504 psia. This large heating requirement of the reboiler is met using high-pressure steam. The high pressure of the bottoms stream must be relieved before it can enter the next column, and a valve is used to reduce the stream’s pressure to 205 psia, which causes a subsequent temperature increase to 442 °F.

The liquid stream, still composed primarily of butadiene and NMP, is fed on stage 20 of the next, 35-stage, column (D-404). Additional NMP is fed to the top of the column. This column separates butadiene from 1-butene, which is a notoriously difficult separation. Initially, it was found that absolutely pure NMP was required to meet the necessary purity (99.5% by weight) of the butadiene product. After careful optimization, this NMP requirement has been reduced, and thus recycled NMP of 99.96% purity by weight is fed into the top of the column. This process to optimize this recycle stream will be discussed further in the following section. Using this NMP, it was possible to get a product stream of 99.5% purity by weight 1,3-butadiene in the distillate of the column as a liquid at 191 °F and 200 psia. This product is sent to a storage tank to be sold. The bottoms stream contains primarily NMP and remaining hydrocarbons, mainly 1-butene, and leaves the column at 554 °F and 206 psia. The large heating requirement of the reboiler will be met by high-pressure steam.

The NMP and 1-butene stream is fed into a final column (D-405) in order to separate out high-purity NMP for the purpose of recycling it as the NMP feeds to columns D-402, D-403, and D-404. This separation is trivial, due to the large volatility difference between NMP and the remaining hydrocarbons. The column uses only 5 stages and a maximum pressure of 52.3 psia to recover 99.7% of the fed NMP at a purity of >99.95% by weight. The NMP leaves in the bottoms stream at 504 °F and 52 psia, and the large heating requirement of the reboiler will be met using high-pressure steam. The purified NMP is then split into three recycle streams, which are fed to columns D-402, D-403, and D-404, and a purge stream to keep the system in mass balance. 1% of the NMP is purged to avoid the build-up of byproducts, and the purged NMP can be stored and sold for a markdown due to slight impurities (<0.05% by weight). The distillate of the column leaves as a liquid at 105 °F and 50 psia and contains primarily 1-butene, 1,3-butadiene, pentenes, and NMP. It will be stored in a tank and sold as a gasoline product.

Optimization of Recycle Stream

The separation of 1,3-butadiene is difficult due to the small volatility differences between the hydrocarbon by-products (namely propylene, 1-butene, and cis/trans-2-butene) mixed in the stream. This is why the extractive solvent NMP is used, to increase the volatility difference between 1,3-butadiene and its accompanying hydrocarbons. However, because Aspen seems to model this extractive distillation process imperfectly, many problems arose with the integration of NMP, particularly when it came to recycling NMP with slight impurities. As a result, the original design of the process required pure NMP feed to the third extractive distillation column (D-404) in order to achieve the designated 99.5% by weight purity of 1,3-butadiene. This required 38,134 lb/hr of fresh NMP to the system, while a similar amount of 38,132 lb/hr of NMP with purity of about 99.9% by weight were purged from the system and sold for a $0.25/lb markdown. This significant waste of NMP was a large cost to the system equivalent to about $9,533.50/hr.

In order to increase profitability, it was clearly necessary that this waste of NMP be reduced. Therefore, rigorous methods were taken in order to implement a full NMP recycle to the system. Many different methods on Aspen were attempted, and with the assistance of industrial advisor Stephen Tieri, we explored methods such as: estimating column profiles, changing the NMP purge/addition/recycle stream configuration, adding a global design spec to maintain overall NMP mass balance in the recycle, and specifying convergences for several design specs. Using these methods, a simulation requiring only 1% purge of NMP was finalized.

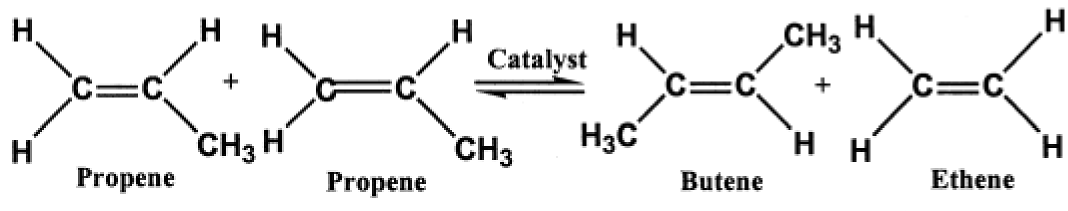
This 1% purge of NMP is absolutely necessary to the system in order to purge trace elements of hydrocarbons such as propylene, 1-butene, and 1,3-butadiene from the recycle and avoid buildup. While purging 1% NMP still requires a fresh NMP feed of about 1367 lb/hr, which, when considering the $0.25 markdown purged NMP must be sold for, still ends up costing $341.80/hr, it is still a considerable improvement. This optimization of the NMP recycle stream will cut overall system costs by $9,191.70/hr, which cuts costs by $72,798,244.20 per year when adjusted for operation days. This was one of our many focuses in order to reduce expenses and optimize our system.

6.0 REACTOR DESIGN

6.1 METATHESIS REACTION

Introduction

The first reaction of the process is the olefin metathesis of propylene to 2-butene. In olefin metathesis, molecules of hydrocarbons are fragmented at the location of their double bonds. These fragments then recombine to form different olefin molecules. The general outline of this process is best described by the below schematic:



Olefin Metathesis

Metathesis reactions are responsive to catalysis, even with very high substrate-to-catalyst ratios, and have the added benefit of attaining equilibrium very quickly, often only taking seconds (Mukherjee, 2006). Over the years, metathesis reactions have been growing in popularity and applicability in industry as more kinetic and thermodynamic information becomes available. The olefin metathesis of propylene to 2-butene, while one of the more common forms of olefin metathesis, still lacks the kinetic and catalytic information to be found in many industrial processes. Therefore, its application in the production of 1,3-butadiene in this process is fairly innovative.

Metathesis reactions are a recent discovery in the chemical industry, with the first uncatalyzed metathesis reaction occurring in 1931. This original reaction required incredibly high temperatures (>1500 °F), and experimentation with catalysts in order to reduce this temperature requirement and improve yield began. Over the years, better catalysts have been created for metathesis processes, making the reaction more feasible for use in many industries. The most recent use of olefin metathesis to produce butenes from propylene was in 1996 by Phillips Petroleum Co. At the time, the process used a WO_3/SiO_2 catalyst doped with sodium at a temperature of 660-800 °F to achieve a 90% yield of 2-butene. However, this process was discontinued in 2002 due to the falling price of butenes and rising cost of propylene.

In our process, we will be looking to develop a new catalyst that improves upon the specifications of the catalyst from the 1996 process. Catalysis technology has developed significantly over the last 19 years, and as a result fairly rigorous catalyst specifications have been chosen in order to optimize the economic feasibility of the process. In general, the main limitations of metathesis processes tend to be low conversion per pass and the occurrence of side reactions. The catalyst to be developed for this process will aim to improve conversion of propylene per pass as well as to limit isomerization side reactions of 2-butenes.

Because this application of olefin metathesis is fairly new in the chemical industry, the kinetic information available is very limited. Instead, to determine the optimal catalyst and reactor conditions, a thorough sensitivity analysis was performed around the metathesis process, and general guidelines from a paper on metathesis technology was used (Mukherjee, 2006).

Determination of Optimal Operating Conditions and Other Operation Considerations

First, optimal operating temperature and pressure of the metathesis process were determined. Metathesis reactions generally have very low energy requirements, as they can be run at very moderate temperatures and tend to generate minimal heat. This is one of the major advantages of the process, and has earned metathesis the reputation of a “green process”. Selectivity analysis on the metathesis of propylene to butenes proved that the reaction is best run at fairly low temperatures. First, the effect of temperature on the production of cis- and trans- 2-butene was analyzed, as these are the main two desired products from the metathesis reaction. It should be noted that because metathesis reactions attain equilibrium so quickly, all values shown here at equilibrium.

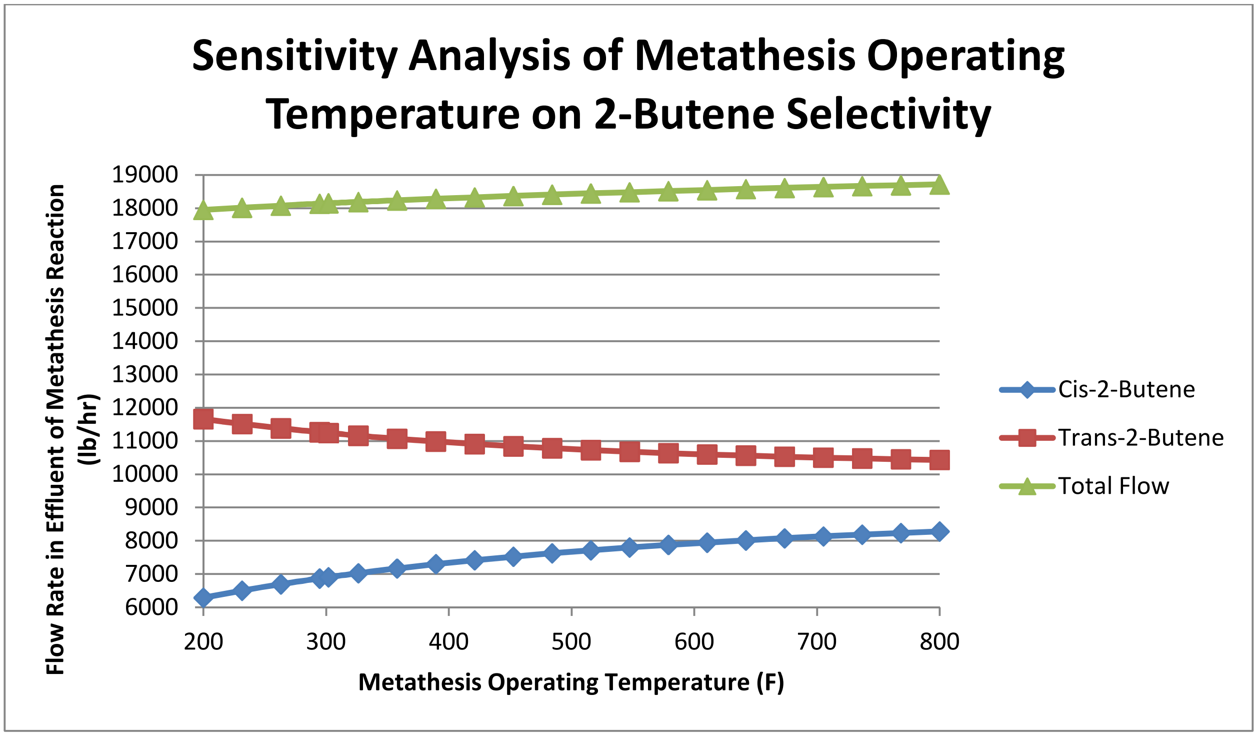


Figure 6.1.1 Sensitivity Analysis of Metathesis Operating Temperature on Selectivity

As can be seen from Figure 6.1.1, the increase in the operating temperature of the metathesis reaction shifts selectivity more in favor of cis-2-butene, while decreasing the equilibrium value of trans-2-butene. Overall, temperature has a slightly positive effect on the total flow rate of 2-butenes, and the conversion of propylene increases from 35.30% at 200 °F to 38.89% at 800 °F.

This information alone favors metathesis at a higher temperature; however, temperature also has an effect on the prevalence of side reactions. Olefin metathesis includes a number of side reactions, most occurring as a result of the isomerization of 2-butene to form less stable, more reactive 1-butene. To determine the types and extent of side reactions, first a reasonable estimate for the isomerization of 2-butene to 1-butene must be made. While some kinetic information is available for this isomerization reaction, it can be assumed that the metathesis catalyst will have a strong effect on the occurrence of side reactions, as that is one of the major purposes of the catalyst. Literature (Happel, et al., 1971) suggests that the isomerization of 2-butene to 1-butene is a highly temperature-dependent process, with the process becoming rapidly more favorable as temperatures extend past 250 °F. Because the lower limit for metathesis tends to be around 250-300 °F, isomerization will likely be unavoidable. Standard isomerization conversions tend to range between 10-20%, and so an isomerization conversion of 10% was suggested to us by our industrial advisor, Gary Sawyer. This is on the lower end of standard isomerization conversions, and it can be assumed that the metathesis catalyst assists in achieving this low conversion of 2-butene.

After determining the 10% conversion of 2-butene to 1-butene via isomerization, the various side reactions that 1-butene may undergo must be taken into account. These side reactions include:

1. Isomerization of 2-Butene to 1-Butene:

   $C_4H_8\text{-}2 \rightarrow C_4H_8\text{-}1$

2. Formation of Pentenes (cis and trans):

   $C_4H_8\text{-}1 + C_3H_6\text{-}2 \rightarrow C_2H_4 + C_5H_{10}\text{-}2$

3. Formation of Hexenes (cis and trans):

   $2C_4H_8\text{-}1 \rightarrow C_2H_4 + C_6H_{12}\text{-}3$

The sensitivity of these side reactions to temperature was examined in order to determine the optimal operating conditions for the reactor, and it was found that the mass flow rate of these byproducts increased with temperature, primarily due to the production of additional cis-2-pentene.

These side reactions are undesirable in our process for a variety of reasons: (1) they consume additional propylene, our feed material, which is one of the largest costs to our process; (2) they make the separation of 2-butene through distillation more difficult; and (3) the side reactions are endothermic and increase the steam requirement for the reaction vessel.

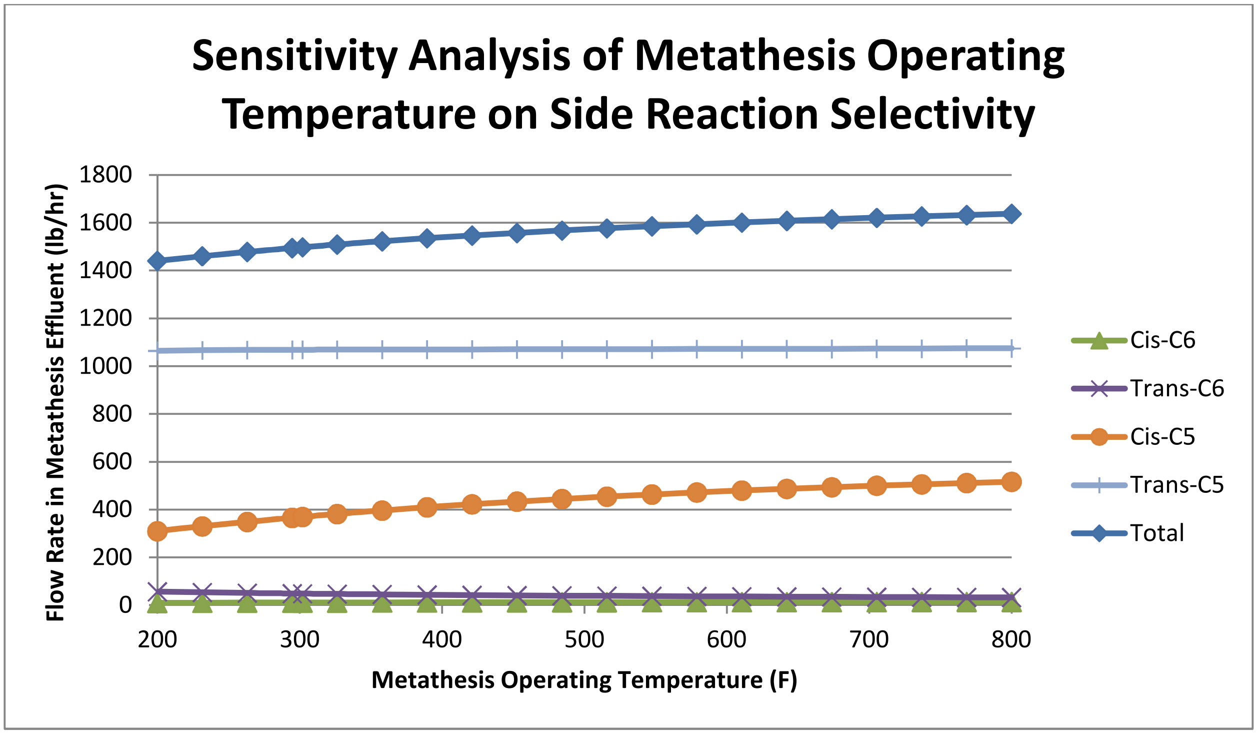


Figure 6.1.2: Sensitivity Analysis of Metathesis Operating Temperature on Side Reaction Selectivity

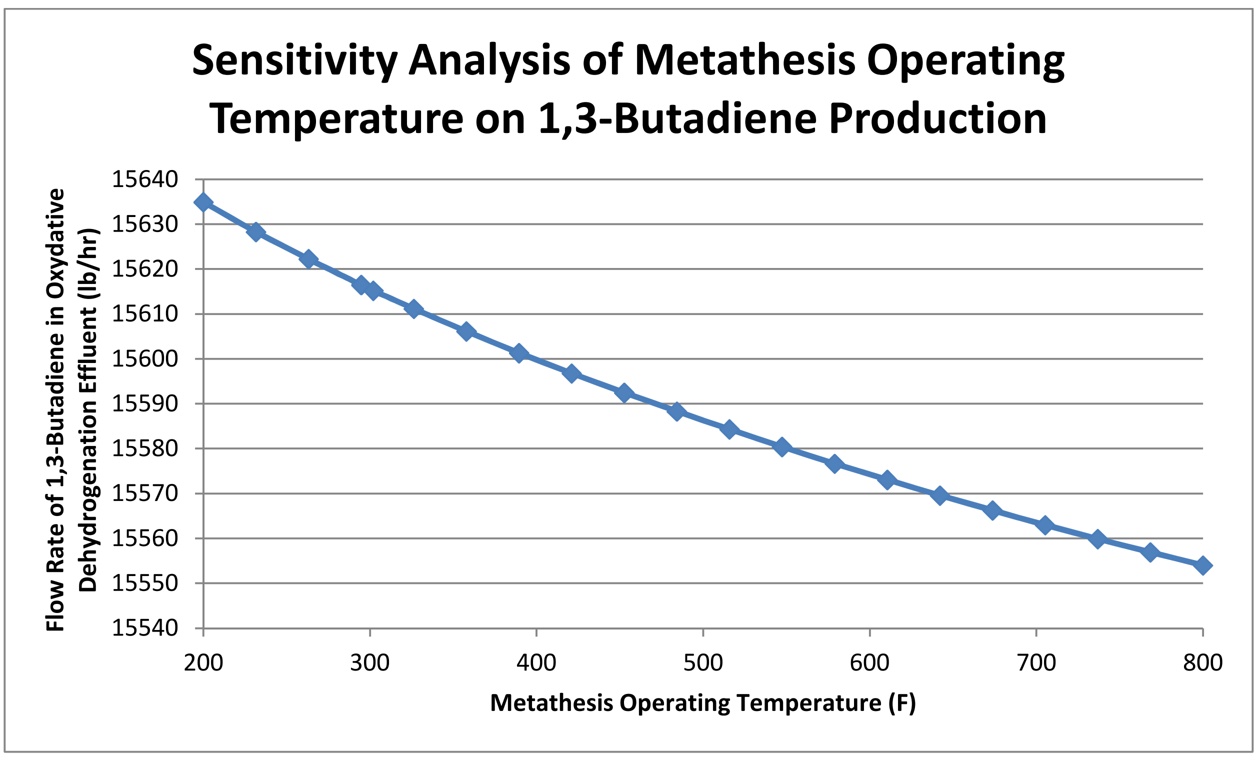


Figure 6.1.3: Sensitivity Analysis of Metathesis Operating Temperature on 1,3-Butadiene Production

Furthermore, when the effect of increasing reactor temperature was analyzed in terms of 1,3-butadiene production, it was discovered that the production of 1,3-butadiene decreases, though marginally, with temperature. While this may seem to contradict the results pointing to an increase in production of 2-butene and conversion of propylene with temperature, upon further analysis it became clear that the temperature-dependent shift toward cis-2-butene increases the difficulty of separating the 2-butenes from unreacted propylene prior to oxidative dehydrogenation.

As the mass flow rate of cis-2-butene in the reactor effluent increases, so does the percentage of 2-butenes entering the recycle from distillation column D-202. Particularly, the fraction of cis-2-butene leaving the column in the recycle increases as the flow rate of cis-2-butene increases. Therefore, because increasing temperature makes the metathesis process more selective toward cis-2-butene, and because more cis-2-butene is then lost during separation, the mixed 2-butene feed to the oxidative dehydrogenation reactor actually decreases with the metathesis operating temperature, and this decrease in 2-butene feed leads to a decrease in 1,3-butadiene production.

Considering both the increase in byproducts and the decrease in 1,3-butadiene production as temperature increases, it is clear that the temperature of the metathesis process should be kept fairly low to optimize the process. From the literature, the approximate minimum temperature for metathesis is generally in the range of 250-300 °F, and so to remain slightly above this the operating temperature of 302 °F was chosen for the reactor.

The effect of pressure on the metathesis process was also explored, and from the sensitivity analysis it was determined that the metathesis reaction is fairly independent of pressure, and therefore a low pressure was chosen to minimize compression and pumping costs. In order to keep the pressure high enough to keep the system flowing, however, a pressure slightly above atmospheric was necessary, and so the pressure of 29 psia was chosen for the metathesis process. Figure 6.1.4 and Figure 6.1.5 show the effect of pressure on both the production of 2-butenes and the selectivity of the side reaction, and it is clear that any deviations due to pressure are obsolete.

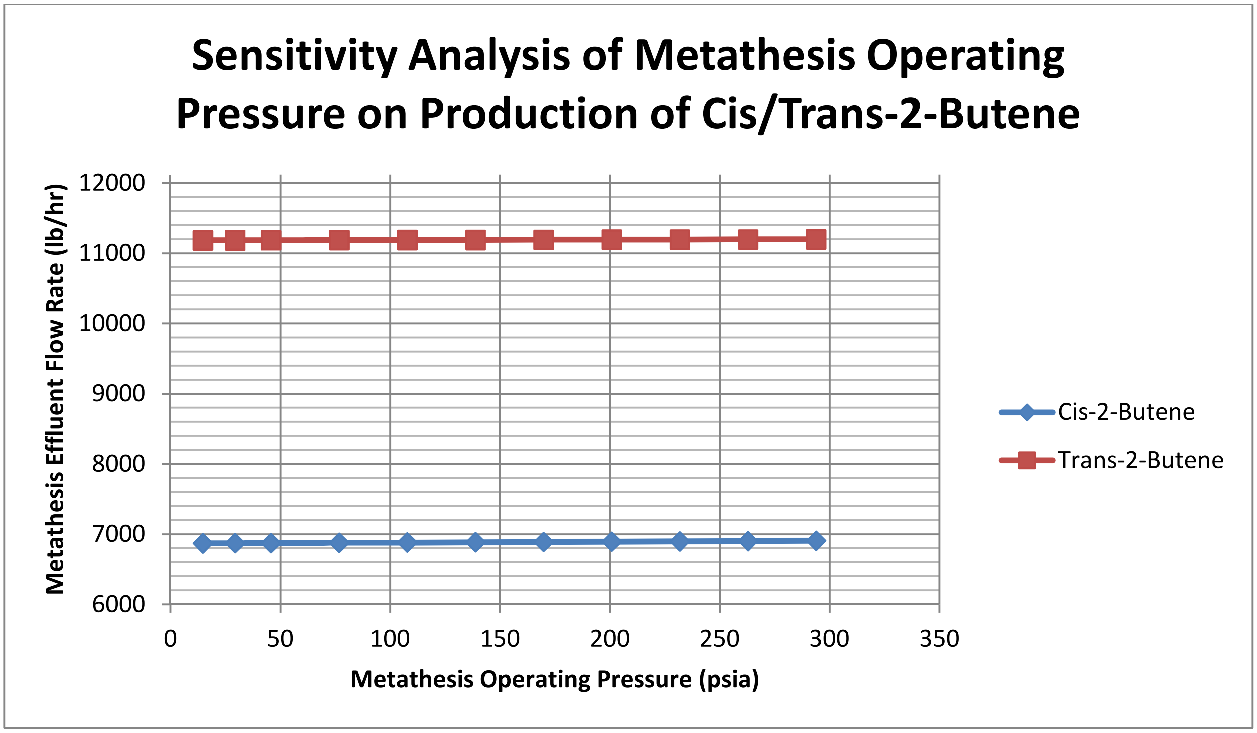


Figure 6.1.4: Sensitivity Analysis of Metathesis Operating Pressure on Production of Cis/Trans-2-Butene

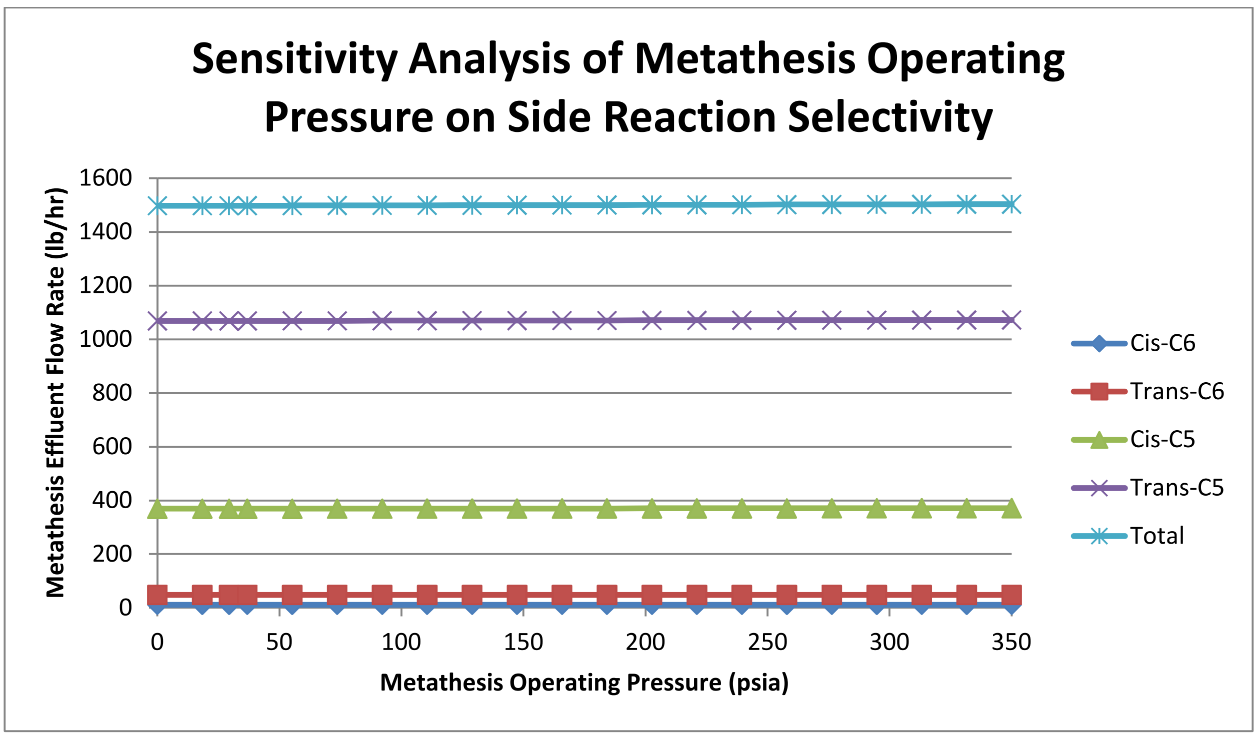


Figure 6.1.5: Sensitivity Analysis of Metathesis Operating Pressure on Side Reaction Selectivity

The conclusion from the sensitivity analysis was that the optimal operating conditions in the metathesis reactor for production of 1,3-butadiene through metathesis is a temperature of 302 °F and a pressure of 29 psia. These operating conditions limit side reactions while keeping the production of 1,3-butadiene and conversion of propylene high. In addition to choosing the optimal operating conditions, the specifications of the catalyst for this process will also help to optimize production.

Metathesis Catalyst Design

In industry today, the reverse of the metathesis process seen here is used. This industrial process uses 2-butene to break into two propylene molecules, and based on the conversion of this reverse reaction, we were told to expect a conversion per pass of propylene of about 15%. This low conversion presented a serious limitation to our process, and the most important job of the catalyst to be developed for this metathesis reaction is that it must improve the conversion per pass of propylene. Using this understanding as a basis for our process design, we used Aspen to optimize the conversion of propylene per pass. By using a combination of Requil and Rstoic blocks in Aspen to model the process as ideally as possible, we managed to model the metathesis process at 36.24% conversion of propylene. This is considerably higher than the expected conversion capacity of the process, and therefore the main design specification for the catalyst will be to achieve this high conversion, even at the fairly low (302 °F) operating temperature of the metathesis unit.

The metathesis should also be optimized to limit side reactions. As part of the metathesis sensitivity analysis, the effect of the isomerization of 2-butene to 1-butene on the final production of 1,3-butadiene was mapped. As can be seen in Figure 6.1.6 below, the isomerization of 2-butene leads to a significant loss in 1,3-butadiene product, especially when the side reaction reaches conversions above 3%. At the current operating capacity of 10%, over 1,000 lb/hr of 1,3-butadiene are being lost due to the isomerization reaction. Because 10% is already on the lower bound of current realistic conversion values, we chose to maintain that fairly significant side reaction conversion. Ideally, however, a catalyst would also be optimized to reduce the isomerization of 2-butenes to 1-butene, and increase selectivity for cis/trans-butenes, which are the desirable products from this process. Limiting the isomerization reaction will in turn limit the presence of reactive 1-butene in the process, thereby limiting the other side reactions to pentenes and hexanes as well.

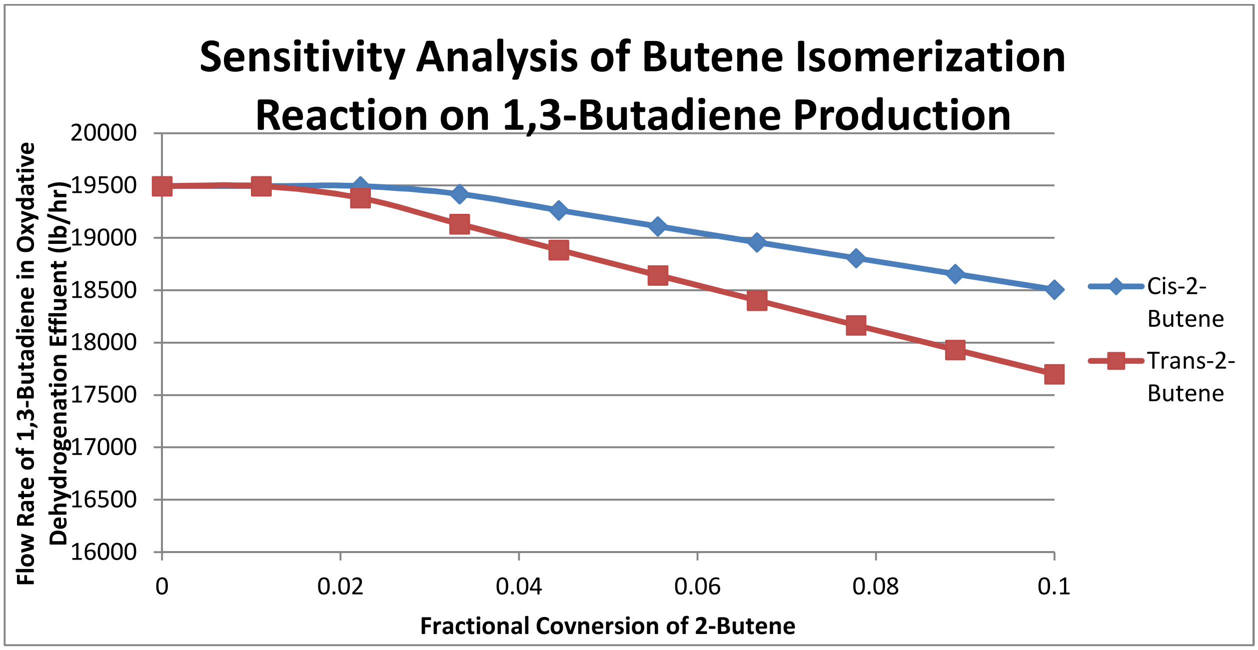


Figure 6.1.6: Sensitivity Analysis of Butene Isomerization Reaction on 1,3-Butadiene Production

In constructing a catalyst of these design specifications, a good starting point would be from the WO_3/SiO_2 catalyst doped with sodium used by Phillips Petroleum Co. in their 1996. Based on suggestions by our industrial consultant Gary Sawyer, it may also be worthwhile looking into tungsten catalysts over silicon. The design should target a high conversion of propylene, particularly 36.24% or above, as well as to attempt to limit the isomerization of 2-butene to 1-butene to a conversion of <3%. While these specifications are rigorous, they will lead to the most optimal process design.

Reactor Flow Rate Calculation and Sizing

The reactor is best designed as a packed bed reactor to allow maximum interaction with the catalyst particles. Its size and price can be determined by first deciphering the volume of the bed. The feed of propylene through the metathesis process is 104,260 lb/hour. Based on our problem statement, a space velocity of 20 kg feed/ kg catalyst/ hour was provided. The volume of the reactor was calculated by dividing the mass flow rate of the propylene feed by the space velocity and density of the feed. This gave a volume of 34,045 ft ^{3} for the reactor. Since, this volume was large and a single reactor would have to be 120 feet or higher, it was decided to split the reaction between two smaller towers. This was also a mechanical advantage as it prevented the possible crushing of the catalyst. It would also decrease the time for catalyst regeneration. A third reactor was added to ensure production does not stop during catalyst regeneration.

Research indicated that packed beds were typically shorter and wider than regular distillation columns; a 1:2.5 diameter to height ratio was selected. Based on this relationship and the volume of the packed bed, a bed height of 52 ft and a diameter of 20 ft was selected. 14 ft were then added to account for spacing at the top and bottom (4 ft each) and and two manholes (3 ft). This lead to a total tower height of 66 ft. Based on these dimensions, the Ergun Equation was used to calculate the pressure drop across the bed. Some assumptions made were of a perfectly spherical catalyst particle with a void fraction of 0.4 and particle diameter of ¼ inch. A low superficial velocity of 0.56 ft/s lead to a small pressure drop of 0.15 psia across the column.

Using the equations in Seider et al and the calculation spreadsheet, a purchase cost of $296,000 was established as the purchase price of one reactor. The total bare module cost for all three reactors is $3,705,200. The number of distributors per reactor was set at 2 to ensure maximum catalytic function. In our project design, three reactors are suggested so that two reactors are always running even when catalyst regeneration or maintenance has to occur. This ensures that the required amount of 2-butene is produced continuously and that there are no holdups in the process

Catalyst Requirements and Regeneration

It is difficult to make accurate assumptions regarding the catalyst, as it is not in commercial or industrial practice nor do we know its physical components. The problem statement provided us with a space velocity and by dividing the mass flow rate through the process by the space velocity; we were able to calculate a volume of catalyst needed. 5313 lbs of catalyst are needed for this reaction. Since we have three reactors, the total volume of catalyst needed is 7819 lbs. Based on the advice of our industrial consultant, Mr. Sawyer, a price of $10/lb was decided for the catalyst. This amounts to $78,920. If we assume that the catalyst has a life span of 2 years, this catalyst would be a $39,460 annual cost.

After the catalyst is in use for some time, coke builds up on the surface of the catalyst and it needs to be fed air diluted with nitrogen for removal purposes. Typically, a carefully controlled combustion reaction with 0.5 vol % oxygen is introduced into the packed bed after it has been purged and dried with Nitrogen at 700 F and a reactor pressure of 60-100 psia. The oxygen concentration can be increased to 2.0 vol% but extreme care should be taken to avoid high temperatures. Depending on the catalyst, it could take from 3-7 days to de-coke. This is why a third reactor has been designed into our process, it prevents a bottleneck being formed in our process due to catalyst regeneration. The life span of the catalyst before regeneration is not known but a starting estimate is 2-3 weeks. The chemist should try and develop a catalyst with a longer life span and short regeneration time. (Handbook of Commercial Catalysts: Heterogeneous Catalysts by Howard F. Rase)

6.2 OXIDATIVE DEHYDROGENATION

Introduction

Oxidative dehydrogenation is a well-known industrial process, often used for converting 2-butenes to 1,3-butadiene. The reaction mechanism works by utilizing oxygen to facilitate the removal of two hydrogen atoms from 2-butene in order to form an additional double bond, resulting in a molecule of 1,3-butadiene and a molecule of water. This process has a large advantage over the non-oxidative process in that it achieves 100% conversion of 2-butenes and high yields of 1,3-butadiene, all at relatively lower temperature.

In order to achieve these high conversions and yields, a catalyst must be used to facilitate the reaction. A variety of catalysts will work for this, with the traditional option being a ferrite catalyst, and over recent years a number of catalysts have been developed to achieve even higher yields of 1,3-butadiene. Recent patent research uses multimetal oxide catalysts to achieve yields of 1,3-butadiene above 90% (Josch et al., 2014).

Two primary reactions occur inside this reactor, one being the desired oxidative dehydrogenation of 2-butenes to 1,3-butadiene, and the second being the undesired combustion reaction of 2-butenes to produce CO_2 and water. The stoichiometry of these reactions is as below:

1. Oxidative dehydrogenation of 2-butenes (cis and trans) to 1,3-butadiene:
    a. $C_4H_8\text{-}2 + 0.5\ O_2 \rightarrow C_4H_6 + H_2O$
2. Combustion of 2-butenes:
    a. $C_4H_8\text{-}2 + 6\ O_2 \rightarrow 4\ CO_2 + 4\ H_2O$

Determination of Optimal Operating Conditions and Other Operation Considerations

In order to determine the optimal operating conditions for the oxidative dehydrogenation, the effect of the side reaction on production of 1,3-butadiene must be considered. A sensitivity analysis was performed, examining the effect of the combustion side reaction on effluent composition as conversion ranged from 0 to 50%. The results of this analysis can be seen in Figure 6.2.1 below, and it is clear that the consumption of oxygen and production of carbon dioxide are the most drastically affected.

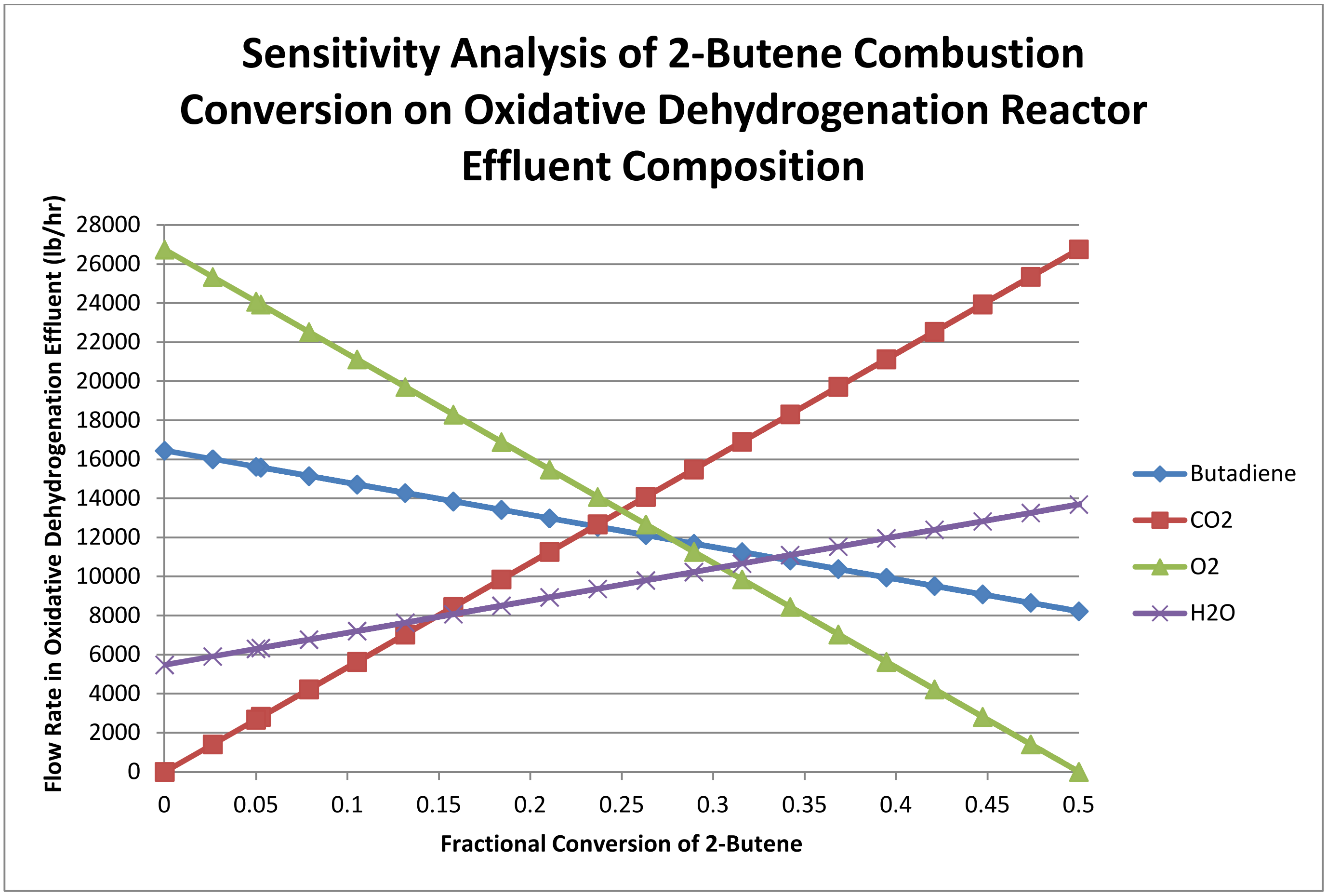


Figure 6.2.1 Sensitivity Analysis of 2-Butene Combustion Conversion on Oxy-D Reactor Effluent Composition

It should also be noted that while Figure 6.2.1 shows the relationship between oxygen consumption and the fractional conversion of 2-Butene combustion, the inlet flow rate of air will be adjusted to maintain a minimal flow rate of oxygen in the reactor effluent, with only a 0.5% excess of oxygen being required. Therefore, the inclusion of the flow rate of oxygen in Figure 6.2.1 was only to display the drastic increase in oxygen required as fractional conversion increases.

The combustion of 2-butene clearly has a negative effect on the flow rate of 1,3-butadiene in the oxidative dehydrogenation effluent, as well as producing more carbon dioxide and water, and requiring a greater amount of oxygen. These are all very undesirable results, as both carbon dioxide and water are undesirable byproducts that must later be separated out of the process. Because air will be used to provide oxygen, increasing the requirement of oxygen significantly increase the volume of air that must be compressed, which in turn increases both utility costs as well as the cost of the compressor. The decrease in 1,3-butadiene production is clearly undesirable, as its production is our primary process goal. Based on these results, minimizing the conversion of 2-butene in the combustion side reaction is advantageous, and therefore conditions should be chosen to achieve this effect.

Based on patent information (Josch et al., 2014), the optimal temperature range for the oxidative dehydrogenation process is between 660 and 790 °F. Kinetic information on the reaction indicates that as temperature increases, so does the yield of 1,3-butadiene up to a point, around 800 °F, where the combustion reaction begins to rapidly increase in favorability and the yield of 1,3-butadiene actually decreases. Based on this kinetic information and suggestions by our industrial consultant, Gary Sawyer, who told us that at 752 °F the fractional conversion for 2-butene combustion would be about 5%, we chose this as the optimal operating condition. This gives a fractional conversion of 95% for 2-butene to 1,3-butadiene, considering that standard total conversions for 2-butene are usually 100%. Any conversion above 90% for 2-butene to 1,3-butadiene is considered good, and to achieve a conversion above 95% would be very difficult and likely require new catalyst development. Therefore, it was decided that a conventional catalyst would be used and the reactor would be operated at a temperature of 752 °F.

The oxidative dehydrogenation reaction is fairly pressure independent, and in fact often low pressures are used to ensure that all components remain in the vapor phase, which is necessary for the reaction. Based on patent specifications, the pressure of 44 psia was chosen. This pressure is just high enough to aid in the flow of components through the reactor and to compensate for any pressure drops that may be encountered while keeping the operating pressure low.

For the oxygen feed to the reactor, it was decided to use air. Patent specifications indicate air as an optimal choice, as the fraction of oxygen in the gas feed should not exceed 30% by volume. A gas feed too high in oxygen content risks diluting the system in oxygen, which increases the occurrence of combustion and other side reactions. The patent therefore recommends an oxygen fraction between 20% and 30% by volume, with air being within that range. Air also has the added benefit of having no upfront cost, and the presence of nitrogen as an inert helps to absorb some of the heat generated during the highly exothermic reaction in order to keep the reactor from overheating.

The reactions occurring in the oxidative dehydrogenation reactor release large amounts of energy, with heats of reactions of:

Reaction	**Conversion**	**Heat of Reaction (Btu/lbmol)**
C_4H_8-2 (cis) + 0.5 $O_2 \rightarrow C_4H_6$-4 + H_2O	95%	-53,881
C_4H_8-3 (trans) + 0.5 $O_2 \rightarrow C_4H_6$-4 + H_2O	95%	-52,333.5
C_4H_8-2 (cis) + 6 $O_2 \rightarrow$ 4 CO_2 + 4 H_2O	5%	-1,089,600
C_4H_8-3 (trans) + 6 $O_2 \rightarrow$ 4 CO_2 + 4 H_2O	5%	-1,088,050

The overall heat duty of the vessel is -3.112 x 10^7 Btu/hr. In order to keep the vessel from overheating and maintain it at its isothermal operating temperature of 752 °F, the vessel must be cooled using cooling water.

Reactor Flow Rate Calculation and Sizing

Based on our literature search, this reactor is best modeled as a fixed bed shell and tube packed bed reactor. The patent suggests using 5,000-30,000 tubes, which are 10-30 mm in diameter with a wall thickness of 1-3mm. The length of the reaction tubes is frequently between 2.5-6m. Keeping these measurements in mind, a 3/4 inch 14 BWG tube has been chosen, that has a flow area per tube of 0.268 $in^{2.}$ Assuming a contact time of 5 s and a tube length of 4m, the volumetric flow rate through one tube is 8.4 in^3/s. The total number of tubes is calculated by the volumetric flow rate of being fed into the reactor divided by the flow rate into one tube. This gives is 7,172 tubes, which is acceptable within the patent limits.

Now, the volume of the entire bed needs to be calculated for sizing purposes. The flow rate through the oxidative dehydrogenation process is 19,687 lb/hour. Based on our problem statement, a space velocity of 1.5 kg feed/ kg catalyst/ hour was provided. The volume of the reactor was calculated by dividing the mass flow rate of the 2-butene feed by the space velocity and density of the feed. This gave a volume of 22,066 ft ^{3} for the reactor. A 1:3.5 diameter to height ratio was selected. Based on this relationship and the volume of the packed bed, a bed height of 72 ft and a diameter of 20 ft was selected. 11 ft were then added to account for spacing at the top and bottom (4 ft each) and two manholes (3 ft each). This lead to a total tower height of 86 ft. Based on these dimensions, the Ergun Equation was used to calculate the pressure drop across the bed. Some assumptions made were of a perfectly spherical catalyst particle with a void fraction of 0.4 and particle diameter of ¼ inch. A low superficial velocity of 0.02 ft/s lead to a small pressure drop across the column.

Using the equations in Seider et al and the calculation spreadsheet, a purchase cost of \$442,900 was established as the purchase price of one reactor. As with metathesis, coke formation on the catalyst is a concern, therefore an additional tower is constructed to ensure the smooth and continuous operation of the process. The total bare module cost for both reactors is \$3,684,000. The number of distributors per reactor was set at 4 to ensure maximum catalytic function.

Catalyst Requirements and Regeneration

The catalyst used for oxidative dehydrogenation is a multimetal oxide the molecular formula $Mo_{12}BiFe_{0.1}Ni_8ZrCr_3K_{0.2}O_{53}$. This is one of the newest catalysts developed for the oxidative dehydrogenation of 2-butenes to 1,3-butadiene (Josch et al., 2014) and is highly selective for 1,3-butadiene, both limiting the occurrence of side reactions as well as maximizing conversion of 2-butenes to 100%.

The catalyst is spherical with a diameter of about 4 mm and a density of about 3.66 g/cm^3. Catalyst life is recommended around 2-3 years with proper occasional treatment. In this case, the catalyst will be treated every 6 months by a pure steam flow rate to remove carbon deposition that forms as a result of combustion. This converts organic deposits to carbon monoxide and dioxide. After regeneration, the catalyst must be reduced with a hydrogen-containing gas.

The time required for regeneration often varies, and literature (S·克罗内 et al., 2007) recommends washing with steam until carbon dioxide and carbon monoxide are present in only trace amounts (<40 ppm) in outlet steam, usually around 4-5 days. A 24-hour wash period with hydrogen-containing gas is then recommended before the catalyst is ready for use again. With this rigorous regeneration schedule, catalyst life should be sustained into 3 years, and thus the recommendation is to replace the catalyst every 3 years.

In order to sustain production during catalyst regeneration and replacement periods, a second reactor vessel must be purchased, and production will be rotated between vessels whenever one needs maintenance.

The volume of catalyst needed can be calculated. The problem statement provided us with a space velocity of 1.5 kg feed/kg catalyst/hour. By dividing the mass flow rate of the 2-butene feed through the process by the space velocity; we were able to calculate a volume of catalyst needed. 13,125 lbs of catalyst are needed for this reaction. Since we have two reactors, the total volume of catalyst needed is 26,250 lbs. Based on our research; the price of the catalyst is $0.295/lb. This amounts to $7,742. This catalyst will typically last for three years, therefore the cost per year is $2580.

7.0 ENERGY

7.1 ENERGY BALANCES

Energy Balances for each of the sections outlined above. It can be seen that oxidative dehydrogenation is very exothermic and generates the most heat in the process. Methods including the use of heat exchangers have been used integrate and redistribute that energy.

Table 7.1.1: Energy Balance for Section 100: Metathesis

METATHESIS				
COMPONENT Flow (lbmol/hr)	**Inlet**		**Outlet**	**Difference**
	S-101	**S-205**	**S-201**	
PROPYLENE	33665	52607	53315	-32957
ETHYLENE	0	14	11595	11581
TRAN-2-BUTENE	0	10128	20231	10103
CIS-2-BUTENE	0	5303	12431	7128
1-BUTENE	0	2442	3691	1248
CIS-C6	0	0	23	23
TRANS-C6	0	0	96	96
CIS-C5	0	24	739	715
TRANS-C5	0	73	2136	2063
TOTAL MASS FLOW (lb/hr)	**33665**	**70593**	**104258**	**0**
ENTHALPY (MMBtu/hr)	**1.503**	**1.19**	**15.66**	**12.96**

Table 7.1.2: Energy Balance for Section 200: Distillation

DISTILLATION						
COMPONENT Flow (lb/hr)	**Inlet**	**Outlets**				**Difference**
	S-201	**S-202**	**S-205**	**S-208**	**S-209**	
PROPYLENE	53315	176	52607	532		**0**
ETHYLENE	11595	11581	14			**0**
TRAN-2-BUTENE	20231		10128	10017	86	**0**
CIS-2-BUTENE	12431		5303	7033	96	**-1**
1-BUTENE	3691		2442	1244	4	**1**
CIS-C6	23				23	**0**
TRANS-C6	96			1	95	**0**
CIS-C5	739		24	213	502	**0**
TRANS-C5	2136		73	647	1416	**0**
TOTAL MASS FLOW (lb/hr)	104257	11757	70593	19687	2220	**0**
ENTHALPY (MMBtu/hr)	7.256	1.191	15.655	-3.932	-0.589	**-5.07**

Table 7.1.3: Energy Balance for Section 300: Oxidative Dehydrogenation

OXIDATIVE DEHYDROGENATION				
COMPONENT Flow (lbmol/hr)	**Inlets**		**Outlets**	**Difference**
	S-209	**S-302**	**S-401**	
PROPYLEN	532	0	532	**0**
ETHYLENE				**0**
TRAN-BUT	10017			**10017**
CIS-BUT	7033			**7033**
1-BUTENE	1244		1244	**0**
CIS-C6				**0**
TRANS-C6	1			**1**
CIS-C5	213		213	**0**
TRANS-C5	647		647	**0**
OXYGEN		7566	31	**7535**
CARBON DIOXIDE			2675	**-2675**
NITROGEN		24919	24919	**0**
1:3BUTAD			15615	**-15615**
H20			6296	**-6296**
TOTAL MASS FLOW lb/hr	**19687**	**32485**	**52172**	**0**
ENTHALPY MMBtu/hr	**-3.93**	**-0.07**	**-25.94**	**21.93**

Table 7.1.4: Energy Balance describing Section 400: Extractive Distillation

EXTRACTIVE DISTILLATION										
COMPONENT Flow (lb/hr)	Inlets		Outlets							Difference
	S-308	S-418	S-405	S-407	S-409	S-410	PRODUCT	S-415	PURGE	
PROPYLEN	532			372	105	16	38			**1**
1-BUTENE	1244				2	0	57	1185		**0**
1:3BUTAD	15615			328	913	384	13039	951		**0**
CO2	2675			2538	132	4				**1**
O2	31			30						**1**
N2	24919			24660	258	1				**0**
H20	6296		6286					9		**1**
TRANS-C6	1		1							**0**
CIS-C5	213		5					208		**0**
TRANS-C5	647		12					635		**0**
NMP		1828				28	14	418	1367	**1**
TOTAL MOL FLOW lbmol/hr	**52172**	**1828**	**6304**	**27930**	**1411**	**433**	**13149**	**3405**	**1368**	**0**
ENTHALPY MMBtu/hr	**-25.94**	**-2.10**	**-41.13**	**-10.07**	**0.38**	**0.27**	**10.19**	**-0.32**	**-1.29**	**13.95**

7.2 Utilities

Overview:

This plant uses electricity, steam for heating streams, and cooling water, chilled water, and propane for cooling streams. The cost for each utility is summarized below in table 7.2. The total utility expenditure per year is approximately $22.8 million. Costs were estimated using the values in Seider et al. in conjunction with Aspen's utility calculator. Heat and electricity was redistributed in order to reduce costs, but utilities were still the highest cost in the process.

Table 7.2: Summary of Utility costs

Utillity	Annual Cost
Electricity	$1,829,394.31
Steam	$12,401,898.04
Cooling Water	$355,455.51
Chilled Water	$169,775.40
Propane	$8,081,511.53
Total	**$22,838,034.78**

7.2.1 Electricity

Electricity is required to power all pumps and compressors in the process. Using an estimation of $0.06/kWh, a table of electricity requirements for all pressure changers was constructed and displayed below in table 7.2.1.

Table 7.2.1: Electricity Utility Requirements

Utility Type	Equipment	ID	Usage (kW-h)	Cost ($/hr)
ELECTRICITY	PUMP	P-101	37.57	$2.25
	PUMP	P-201	14.66	$0.88
	PUMP	P-202	4.78	$0.29
	PUMP	P-401	39.35	$2.36
	PUMP	P-402	39.35	$2.36
	PUMP	P-403	12.14	$0.73
	COMPR	C-101	2004.25	$120.25
	COMPR	C-301	704.25	$42.26
	COMPR	C-401	993.38	$59.60
	Total Annual Cost			**$1,829,394.31**

Most of the electricity requirement comes from the compressors compressing the vapor streams of up to 500 psi. Electricity usage was minimized by using a multistage compressor for C-101 which reduced its electricity requirements by over 50 %, saving total electricity utility costs per year by over $1.1 million. A second multistage compressor was attempted in extractive distillation's C-401, but the work requirement increased when trying the new multistage compressor, so a normal compressor was chosen instead. The electricity usage from all units totals 3850 kWh which amounts to a total annual cost of approximately $1.83 million.

7.2.2 STEAM

To calculate the steam requirement for the process, 2 standard types of steam were used: high pressure and low pressure saturated steam at pressures of 50 psi and 450 psi. In every heat intensive unit, heat exchangers, reboilers, and reactors, the heat duty and usage were determined in Aspen and provided in table 7.2.2 below. An example calculation of usage determination can be found in appendix B.

Table7.2.2: Steam Utility Requirement for the Process

Utility Type	Equipment	ID	Usage (lbs/hr)	Duty (Btu/hr)	Cost ($/hr)
50 PSI STEAM	REBOILER	D-201	33500	30600000	$100.61
	REBOILER	D-202	18900	17200000	$56.71
	REBOILER	D-203	4680	4260000	$14.03
	REBOILER	D-402	4540	4140000	$12.13
	REACTOR	R-101	7750	7070000	$23.26
	REACTOR	R-102	100	131000	$0.43
	REACTOR	R-103	25	22800	$0.08
	REACTOR	R-104	7750	7070000	$23.26
	REACTOR	R-105	100	131000	$0.43
	REACTOR	R-106	25	22800	$0.08
450 PSI STEAM	REBOILER	D-401	4050	3102000	$26.73
	HEAT EX	H-301	4790	3671000	$31.63
	HEAT EX	H-303	100000	89100	$657.61
	REBOILER	D-403	9520	7289000	$61.67
	REBOILER	D-404	33820	25910000	$220.58
	REBOILER	D-405	51200	39220000	$336.66
	Total Annual Cost				**$12,401,898.04**

The heating requirements from steam were immense because of the high temperatures the reboilers of the distillation columns need to achieve. Costs were calculated using a value of $0.003 per pound of 50 psi steam and $0.0066 per pound of 450 psi steam. Expenditures for steam were spared by using heat exchangers to take the heat generated from the metathesis and oxidative dehydrogenation reactors to internally heat streams into hotter units. An example of this can be seen in H-101 where the heat generated from the compressed stream out of the metathesis reactors is exchanged with the heat coming into the reactors. By using the heat generation throughout the process, less steam was required which also corresponds to more money saved. The total steam required for the process is 45.7 million pounds of steam per year at a total annual cost of $12.4 million.

7.2.3 Cooling Water

Many streams, such as reactor effluents and tower distillates require cooling water to cool the stream into the next unit or to condense a vapor in a total condenser. Cooling water is available at 90 F as a feed and was taken as an outlet in this process at a maximum temperature of 120 F. The cost for the cooling water was taken as $0.075/1000 gallons. The requirements for cooling water are summarized below in table 7.2.3.

Table 7.2.3: Summary of cooling water utility requirements for the process

Utility Type	Equipment	ID	Usage (lbs/hr)	Duty (Btu/hr)	Cost ($/hr)
COOLING WATER	FLASH3	F-401	444000	13290000	$5.68
	CONDENSER	D-202	626000	18750000	$8.01
	CONDENSER	D-203	190000	5680000	$2.43
	CONDENSER	D-403	78000	2330000	$1.00
	CONDENSER	D-404	650000	19550000	$8.35
	CONDENSER	D-405	1520000	45440000	$19.41
	Total Annual Cost				**$355,455.51**

The total annual cost of cooling water was determined to be $355,000 at a total usage of 4.3 trillion gal/year for the entire process. However, some columns required distillate temperatures below 90 F in which case either chilled water was used or propane for extremely low temperatures was required.

7.2.4 Chilled Water

Chilled water is the next alternative to cooling water when a cooling requirement goes beyond the lower limit of 90 F. Here, only one column condenser fit the temperature conditions, D-401, and the only alternative refrigerant to satisfy the cooling requirement is propane, which is much costlier. Chilled water is available in the limits of 45 F and 90 F in the process at a cost of $1.20/ton. Using this value provided in Seider, as well as the inlet/outlet conditions stated above, table 7.2.4 was generated summarizing the chilled water requirements for the process.

Table 7.2.4: Chilled water utility requirements for the process

Utility Type	Equipment	ID	Usage (lbs/hr)	Duty (Btu/hr)	Cost ($/hr)
CHILLED WATER	CONDENSER	D-401	1670000	75300000	$21.44
	Total Annual Cost				**$169,775.40**

This total annual cost for chilled water amounted to $170,000 for column D-401 at a total usage of approximately 1000 tons/hour.

7.2.5 Propane

Two columns require a cooling requirement further below the temperature conditions of chilled water. Propane was used as a suitable, but expensive, refrigerant in these two cases. Commercially available at $25.95 per million Btu, propane is fed in at a temperature of -40 F and exits at a maximum temperature of 0 F. This completely satisfies the condensers in columns D-201 and D-401 where temperatures are required to be down to -21 F.

Table 7.2.5: Propane utility requirements for the process

Utility Type	Equipment	ID	Usage (lbs/hr)	Duty (Btu/hr)	Cost ($/hr)
PROPANE	CONDENSER	D-201	1980	39320000	$1,020.39
	CONDENSER	D-402	680	13520000	$350.76
	Total Annual Cost				**$8,081,511.53**

Total propane requirement for the process amounts to 20 million pounds of propane per year and a total annual cost of just over $8 million. This is the most expensive utility in the process and attempts were made to cut down the usage of propane, but the condensers of columns D-201 and D-402 required very low temperatures that could only be satisfied at these rates.

8.0 EQUIPMENT

8.1 EQUIPMENT LIST

Equipment Number	Name	Type
Pumps		
P-201	Centrifugal Pump 2	Process Machinery
P-202	Centrifugal Pump 3	Process Machinery
P-401	Centrifugal Pump 4	Process Machinery
P-402	Centrifugal Pump 5	Process Machinery
P-403	Centrifugal Pump 6	Process Machinery
Compressors		
C-101	Compressor 1	Process Machinery
C-301	Compressor 3	Process Machinery
C-401	Compressor 4	Process Machinery
Distillation Column Components		
D-201-C	Condenser	Fabricated Equipment
D-201-R	Reboiler	Fabricated Equipment
D-201-RP	Reflux Pump	Fabricated Equipment
D-201-RA	Reflux Accumulator	Fabricated Equipment
D-201	Tower	Fabricated Equipment
D-202-C	Condensor	Fabricated Equipment
D-202-R	Reboiler	Fabricated Equipment
D-202-RP	Reflux Pump	Fabricated Equipment
D-202-RA	Reflux Accumulator	Fabricated Equipment
D-202	Tower	Fabricated Equipment
D-203-C	Condensor	Fabricated Equipment
D-203-R	Reboiler	Fabricated Equipment
D-203-RP	Reflux Pump	Fabricated Equipment
D-203-RA	Reflux Accumulator	Fabricated Equipment
D-203	Tower	Fabricated Equipment
D-401-C	Condensor	Fabricated Equipment
D-401-R	Reboiler	Fabricated Equipment
D-401-RP	Reflux Pump	Fabricated Equipment

D-401-RA	Reflux Accumulator	Fabricated Equipment
D-401	Tower	Fabricated Equipment
D-402-C	Condensor	Fabricated Equipment
D-402-R	Reboiler	Fabricated Equipment
D-402-RP	Reflux Pump	Fabricated Equipment
D-402-RA	Reflux Accumulator	Fabricated Equipment
D-402	Tower	Fabricated Equipment
D-403-C	Condensor	Fabricated Equipment
D-403-R	Reboiler	Fabricated Equipment
D-403-RP	Reflux Pump	Fabricated Equipment
D-403-RA	Reflux Accumulator	Fabricated Equipment
D-403	Tower	Fabricated Equipment
D-404-C	Condensor	Fabricated Equipment
D-404-R	Reboiler	Fabricated Equipment
D-404-RP	Reflux Pump	Fabricated Equipment
D-404-RA	Reflux Accumulator	Fabricated Equipment
D-404	Tower	Fabricated Equipment
D-405-C	Condensor	Fabricated Equipment
D-405-R	Reboiler	Fabricated Equipment
D-405-RP	Reflux Pump	Fabricated Equipment
D-405-RA	Reflux Accumulator	Fabricated Equipment
D-405	Tower	
Flash		
F-401	Flash Vessel	Fabricated Equipment
Heat Exchangers		
H-101	Shell and Tube	Fabricated Equipment
H-301	Shell and Tube	Fabricated Equipment
H-302	Shell and Tube	Fabricated Equipment
H-303	Shell and Tube	Fabricated Equipment
Reactors		
R-101	Metathesis Reactor 1	Fabricated Equipment
R-102	Metathesis Reactor 2	Fabricated Equipment

R-103	Metathesis Reactor 3	Fabricated Equipment
R-301-A	Oxydehydrogenation Reactor 1	Fabricated Equipment
R-301-B	Oxydehydrogenation Reactor 2	Fabricated Equipment
Storage Tanks		
T-101	Storage Tank 1	Fabricated Machinery
T-201	Storage Tank 2	Fabricated Machinery
T-202	Storage Tank 3	Fabricated Machinery
T-401	Storage Tank 4	Fabricated Machinery
T-402	Storage Tank 5	Fabricated Machinery

8.2 Unit Descriptions

8.2.1 Pumps

P-201

This pump is a cast iron 3600RPM centrifugal pump used to move the bottoms product between D-201 and D-202. P-201 has a -20 hp net work. The pump is necessary for maintenance and smooth working of the distillation column as there is already a pressure gradient present. The purchase price of P-201 is $8,800 and its installed cost is $29,040.

P-202

Pump P-202 is a cast iron 3600RPM centrifugal pump used to move the bottoms product between D-202 and D-203. P-202 has -6.5 hp net work. The pump is necessary for maintenance and smooth working of the distillation column as there is already a pressure gradient. The purchase price of P-202 is $5,800 and the installation cost is $19,140.

P-401

Pump 401 is a cast iron 3600 RPM centrifugal pump used to increases the pressure of S-426 entering D-402 from 100 psi to 501 psia, since extractive distillation needs to run at a high pressure of 500 psia. The net work required is 54 Hp and the pump efficiency is 0.56. The outlet flow rate is 143 gpm. The purchase cost of the pump is $53,500 and installation cost is $176,550.

P-402

Pump 401 is a cast iron 3600 RPM centrifugal pump used to increases the pressure of S-428 entering D-403 from 100 psi to 501 psia, since extractive distillation needs to run at a high pressure of 500 psia. The net work required is 53 Hp and the pump efficiency is 0.56. The outlet flow rate is 142 gpm. The purchase cost of the pump is $53,500 and installation cost is $176,550.

P-403

Pump 403 is a cast iron 3600 RPM centrifugal pump used to increases the pressure of S-429 entering D-404 from 50 psia to 501 psia, since extractive distillation needs to run at a high pressure of 500 psia. The net work required is 16 Hp and the pump efficiency is 0.56. The outlet flow rate is 109 gpm. The purchase cost of the pump is $17,200 and the installation cost is $56,760.

8.2.2 Compressors

C-101

This is a carbon steel multi-stage compressor used to compress the vapor from the metathesis reaction from 29 psia to 400 psia. This is to ensure the feed to Section 200 of our process is at a stable pressure to enter the distillation. The isentropic efficiency is assumed to be 0.72. The inlet gas flow rate through the compressor is 10873.25 ft^3/min at a pressure of 29.39 psia. The brake power required for the compressor is 5394 hp. At an installed weight of 21,000 lbs, the unit purchase cost is $2.5 million and the bare module cost is $5.3 million.

C-301

This is a carbon steel compressor used to compress air before it is fed to the oxidative dehydrogenation reactor, R-301. The pressure change across the compressor was 35 psia. The isentropic efficiency is assumed to be 0.72. The flow rate through the compressor is 32,485lb/hr. The brake power required for the compressor is 945 hp. With an installed weight of 52,000 pounds, the purchase cost is $1.23 million and the bare module cost is $2.7 million.

C -401

This is a carbon steel compressor used to compress the distillate from D-401 to be fed as a bottoms feed to D-402. The pressure difference across the compressor was 100 psia. The isentropic efficiency is assumed to be 0.72. The flow rate through the compressor is 45,879 lb/hr. The brake power required for the compressor is 1362.8 hp. With an installed weight of 49,000 pounds, the purchase cost is $1.26 million and the bare module cost is $2.7 million.

8.2.3 Heat Exchangers

H-101

Heat Exchanger 101 is a single-pass shell and tube heat exchanger, which receives S-103 at 115 F and releases S-104 at 302 F. The shell is made of carbon steel, and the tube is made of low alloy steel. The heat exchanger heats cools the feed to the distillation section from 574 F to 409 F while heating the metathesis feed, S-104 from 115 F to 302 F. The tube pitch is 1.25 inches, tube length 20 ft, and the effective heat transfer area is 237 square feet. The purchase and installation costs are $14,000 and $42,000 respectively.

H-301

Heat Exchanger 301 is a single-pass shell and tube heat exchanger, which receives compressed air on the tube side that is heated from 372 F to 752F. On the shell side, steam enters at 50 psig.

The tube is made of carbon steel, and the shell made of low alloy steel. On the hot side, the heat exchanger cools and condenses**.** The tube pitch is 1.25 inches, tube length 20 ft and effective heat transfer area is 250 square feet. The purchase and bare module costs are $11,340 and $35,950 respectively

H-302

Heat Exchanger 302 is a single-pass shell and tube heat exchanger, which on the tube side receives stream S-307 at 752 F and releases S-301 at 449 F. The tube is made of low alloy steel and the tube of carbon steel**.** The shell side receives the bottoms from distillation at 143 F in S-208, and gets heated to 485 F before entering F-401 via S-308. The tube pitch is 1.25 inches, tube length 20 ft and the effective heat transfer area is 100 square feet. The purchase and installation costs are $16,040 and $48,120, respectively.

H-303

Heat Exchanger 302 is a single-pass shell and tube heat exchanger, which on the tube side receives stream, receives steam at 50 psia. The tube and shell side is made of low alloy steel**.** The shell side receives the feed to oxydehydrogenation 445 F in S-208, and gets heated to 485 F before entering F-401 via S-308. The tube pitch is 1.25 inches, tube length 20 ft, effective heat transfer area 110 square feet. The purchase and installation costs are $15,200 and $45,600, respectively.

8.2.4 Reactors

R-101

R-101 is a packed bed reactor that allows propylene to form 2-butene and ethylene. Streams enter the reactor at 29 psia and 302 F and leave at the same temperature. The flow rate leaving the reactor sets is 52,130 lb/hr. The pressure drop was calculated using the Ergun Equation and it was found to be 3000 pascals, This low pressure drop makes sense as the superficial velocity is only 0.18 m/s. The height of the reactor is 66ft and the diameter 20ft. The purchase and bare module costs of the reactor are $296,900 and $ 1,235,000, respectively.

R-102

R-102 is a packed bed reactor that allows propylene to form 2-butene and ethylene. Streams enter the reactor at 29 psia and 302 F and leave at the same temperature. The flow rate leaving the reactor sets is 52,130 lb/hr. The pressure drop was calculated using the Ergun Equation and it was found to be 3000 pascals, This low pressure drop makes sense as the superficial velocity is only 0.18 m/s. The height of the reactor is 66ft and the diameter 20ft. The purchase and bare module costs of the reactor are $296,900 and $ 1,235,000, respectively.

R-103

R-102 is a packed bed reactor that allows propylene to form 2-butene and ethylene. Streams enter the reactor at 29 psia and 302 F and leave at the same temperature. The flow rate leaving the reactor sets is 52,130 lb/hr. The pressure drop was calculated using the Ergun Equation and it was found to be 3000 pascals, This low pressure drop makes sense as the superficial velocity is only 0.18 m/s. The height of the reactor is 66ft and the diameter 20ft. The purchase and bare module costs of the reactor are $296,900 and $ 1,235,000, respectively. There are three towers to allow for catalyst regeneration as well as avoiding the possible crushing of the catalyst in one very large reactor. Therefore, the bare module cost of the three identical reactors R-101, R-102, and R-103 is $3,705,200.

R-301

R-301 is split into two reactors, R-301-A and R-301-B. These are packed bed reactors that uses compressed air to convert 2-butene to 1,3-butadiene and water. Streams enter the reactor at 44 psia and 752 F and leaves at the same temperature and pressure. The flow rate leaving the reactor sets is 52,120 lb/hr. The height of the reactor is 86ft and the diameter 20ft. The pressure drop calculated by the Ergun Equation was very low and thus neglected. The purchase and bare module costs of each reactor are $442,900 and $ 1,842,000, respectively

8.2.5 Distillation Columns

D-201

Column D-201 is constructed of carbon steel. The column serves primarily to separate ethylene byproduct from the metathesis effluent at a relatively high purity (98.5% wt). To achieve this, the column uses 20 stages at a height of 63 feet and a diameter of 10.5 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. The feed enters on stage 10. The column operates at a reflux ratio of 26.7 and a pressure of 400 psia. The feed to the column is a 104,261 lb/hr mixture of hydrocarbons at 160 F and 400 psia. Pure liquid distillate leaves the column at a flow rate of 11,756 lb/hr, a temperature of 2.3 F, and a pressure of 400 psia. The bottoms stream leaves the column at a flow rate of 92,504 lb/hr, a temperature of 185.3 F, and a pressure of 403.98 psia. The purchase cost for column D-201 is $495,600 and the bare module cost is $2,061,696.

D-202

Column D-202 is constructed of carbon steel. The column serves primarily to separate unreacted propylene from the metathesis effluent in order to recycle it back to the reactor. To achieve this, the column uses 10 stages at a height of 35 feet and a diameter of 7 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. The feed enters on stage 5. The column operates at a reflux ratio of 1.057 and a pressure of 300 psia. The feed to the column is a 92,500 lb/hr mixture of hydrocarbons at 182.5 F and 300 psia. Pure liquid distillate leaves the column at a flow rate of 70,600 lb/hr, a temperature of 139.3 F, and a pressure of 300 psia. The bottoms stream leaves the column at a flow rate of 21,900 lb/hr, a temperature of 244 F, and a pressure of 302.88 psia. The purchase cost for column D-202 is $149,900 and the bare module cost is $623,584.

D-203

Column D-203 is constructed of carbon steel. The column serves primarily to separate butenes at high recovery (98.99% by wt) and high purity (92.92% by wt) from the remaining side products in the metathesis effluent. To achieve this, the column uses 10 stages at a height of 35 feet and a diameter of 3 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. The feed enters on stage 5. The column operates at a reflux ratio of 0.88 and a pressure of 100 psia. The feed to the column is a 21,908 lb/hr mixture of hydrocarbons at 239.3 F and 103 psia. Pure liquid distillate leaves the column at a flow rate of 2,220 lb/hr, a temperature of 217.3 F, and a pressure of 102.88 psia. The bottoms stream leaves the column at a flow rate of 19,687 lb/hr, a temperature of 142.8 F, and a pressure of 100 psia. The purchase cost for column D-203 is $118,800 and the bare module cost is $494,208.

D-401

Column D-401 is constructed of low alloy steel. The column serves primarily to remove the water in the oxidative dehydrogenation effluent at a high recovery (99.9% by wt) and purity (99.93% by wt). To achieve this, the column uses 10 stages at a height of 35 feet and a diameter of 8 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. There are two feeds to the column; the liquid feed enters on stage 3 and the vapor feed enters on stage 8. The column operates at a reflux ratio of 5 and a pressure of 101 psia. The liquid feed to the column is a 14,325.28 lb/hr mixture at 100 F and 105 psia. The vapor feed to the column is a 37,847.61 lb/hr mixture at 100 F and 105 psia. Pure vapor distillate leaves the column at a flow rate of 45,879.47 lb/hr, a temperature of 63.5 F, and a pressure of 101 psia. The bottoms stream leaves the column at a flow rate of 6,293.43 lb/hr, a temperature of 330.7 F, and a pressure of 103.88 psia. The purchase cost for column D-401 is $136,800 and the installed cost is $569,088.

D-402

Column D-402 is constructed of carbon steel. The column serves primarily to separate non-condensable components (nitrogen, oxygen, and carbon dioxide) from the oxidative dehydrogenation effluent. To achieve this, the column uses 15 stages at a height of 49 feet and a diameter of 4 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. There are two feeds to the column; the solvent feed of NMP enters on stage 2 and the vapor feed enters on stage 15. The column operates at a reflux ratio of 1.0 and a pressure of 500 psia. The solvent feed to the column is 49,549.18 lb/hr of NMP at 506.5 F and 501 psia. The vapor feed to the column is a 45,879.47 lb/hr mixture at 317.6 F and 501 psia. Pure vapor distillate leaves the column at a flow rate of 27,932.56 lb/hr, a temperature of -20.9 F, and a pressure of 500 psia. The bottoms stream leaves the column at a flow rate of 67,496.08 lb/hr, a temperature of 269.3 F, and a pressure of 503.43 psia. The purchase cost for column D-402 is $118,800 and the bare module cost is $494,200.

D-403

Column D-403 is constructed of carbon steel. The column serves primarily to separate remaining propane and non-condensable components from the C_4 hydrocarbons. To achieve this, the column uses 20 stages at a height of 63 feet and a diameter of 4.5 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. There are two feeds to the column; the solvent feed of NMP enters on stage 2 and the liquid hydrocarbon feed enters on stage 15. The column operates at a reflux ratio of 5 and a pressure of 500 psia. The solvent feed to the column is 49,549.18 lb/hr of NMP at 506.5 F and 501 psia. The liquid hydrocarbon feed to the column is 67,496.08 lb/hr at 269.3 F and 503.43 psia. The distillate is split into a liquid and vapor stream; the liquid distillate stream leaves the column at a flow rate of 434.60 lb/hr, and the vapor distillate stream leaves the column at a flow rate of 1,409.05 lb/hr. Both distillate streams exit at a temperature of 226.8F and a pressure of 500 psia. The bottoms stream leaves the column at a flow rate of 115,202 lb/hr, a temperature of 426 F, and a pressure of 503.98 psia. The purchase cost for D-403 is $210,700 and the bare module cost is $876,512.

D-404

Column D-404 is constructed of carbon steel. The column serves primarily to separate 1,3-butadiene product at high purity (99.5% by wt) from the remaining hydrocarbons using NMP. To achieve this, the column uses 35 stages at a height of 96 feet and a diameter of 6.5 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. There are two feeds to the column; the solvent feed of NMP enters on stage 2 and the liquid hydrocarbon feed enters on stage 20. The column operates at a reflux ratio of 10 and a pressure of 200 psia. The solvent feed to the column is 38,165.11 lb/hr of NMP at 101.3 F and 201 psia. The liquid hydrocarbon feed to the column is 115,201.61 lb/hr at 442 F and 205 psia. The purified 1,3-butadiene product exits the system in the liquid distillate, which leaves the column at a flow rate of 13,146.38 lb/hr, a temperature of 190.7 F, and a pressure of 200 psia. The bottoms stream leaves the column at a flow rate of 140,220.34 lb/hr, a temperature of 555.5 F, and a pressure of 205.63 psia. The purchase cost for column D-404 is $331,700 and the bare module cost is $1,380,000.

D-405

Column D-405 is constructed of carbon steel. The column serves primarily to separate NMP at a very high purity (>99.99% by wt) to recycle. To achieve this, the column uses 5 stages at a height of 21 feet and a diameter of 9.5 feet. The tray efficiency was determined to be 70%, and sieve trays were used at a spacing of 2 feet each. The feed enters on stage 5. The column operates at a reflux ratio of 50.7 and a pressure of 50 psia. The feed to the column is a 140,220.34 lb/hr mixture of remaining hydrocarbons and NMP at 555.5 F and 205.63 psia. Pure liquid distillate leaves the column at a flow rate of 3,428.50 lb/hr, a temperature of 105.1 F, and a pressure of 50 psia. The bottoms stream leaves the column at a flow rate of 136,791.84 lb/hr, a temperature of 503.8 F, and a pressure of 52.33 psia. The purchase cost for column D-405 is $103,200 and the bare module cost is $429,300.

8.2.6 Condensers

D-201-C

D-201-C (Figure 200) is a shell-and-tube heat exchanger fabricated from carbon steel. It uses refrigerant with a flow rate of 1980 lb/hr to condense the column overhead from D-201, which has a flow rate of 12,000 lb/hr. This partially condenses the overhead at 2.4 °F and heats the refrigerant, propane from-40 F to 0 F. This process releases 39 MMBTU/hr of heat. The estimated purchase cost is $2,952,000 and the installation cost is $4,720,000.

D-202-C

D-202-C (Figure 200) is a shell-and-tube heat exchanger fabricated from carbon steel. It uses cooling water with a flow rate of 626,000 lb/hr to condense the column overhead from D-202, which has a flow rate of 70,000 lb/hr. This condenses the overhead to 138 °F and heats the cooling water from 90 °F to 120°F. This process releases 18MMBTU/hr of heat. The estimated purchase cost is $86,400 and the installation cost is $274,200.

D-203-C

D-203-C (Figure 200) is a shell-and-tube heat exchanger fabricated from carbon steel. It uses cooling water with a flow rate of 190,000 lb/hr to condense the column overhead from D-203, which has a flow rate of 20,000 lb/hr. This partially condenses the overhead to 142 °F and heats the cooling water from -90 °F to 120 °F. This process releases 5.6 MMBTU/hr of heat. The estimated purchase cost is $28,100 and the installation cost is $89,077.

D-401-C

D-401-C (Figure 400) is a shell-and-tube heat exchanger fabricated from stainless steel. It uses chilled water with a flow rate of 1,950,000 lb/hr to condense the column overhead from D-401, which has a flow rate of 46,000 lb/hr. This condenses the overhead to 58 °F and heats the chilled water, that enters at 45F and exits at 90F. This process releases 75 MMBTU/hr of heat. The estimated purchase cost is $28,100 and the installation cost is $89,077.

D-402-C

D-402-C (Figure 400) is a shell-and-tube heat exchanger fabricated from stainless steel. It uses refrigerant, propane with a flow rate 690 lb/hr to condense the column overhead from D-402, which has a flow rate of 28,000 lb/hr. This condenses the overhead to -25 °F and heats the refrigerant from -40 °F to 0 °F. This process releases 14MMBTU/hr of heat. The estimated purchase cost is $281,500 and the installation cost is $892,400.

D-403-C

D-403-C (Figure 400) is a shell-and-tube heat exchanger fabricated from stainless steel. It uses cooling water with a flow rate of 82,000 lb/hr to condense the column overhead from D-403, which has a flow rate of 11,200 lb/hr. This condenses the overhead to 229°F and heats the cooling water from 90 °F to 120 °F. This process releases 2.3MMBTU/hr of heat. The estimated purchase cost is $9,900 and the installation cost is $41,184.

D-404-C

D-404-C (Figure 400) is a shell-and-tube heat exchanger fabricated from stainless steel. It uses cooling water with a flow rate of 650,000 lb/hr to condense the column overhead from D-404, which has a flow rate of 13,500 lb/hr. This condenses the overhead to 190°F and heats the cooling water from 90 °F to 120 °F. This process releases 19MMBTU/hr of heat. The estimated purchase cost is $40,200 and the installation cost is $127,500.

D-405-C

D-405-C (Figure 400) is a shell-and-tube heat exchanger fabricated from stainless steel. It uses cooling water with a flow rate of 1,530,000 lb/hr to condense the column overhead from D-405, which has a flow rate of 176,000 lb/hr. This condenses the overhead to 105°F and heats the cooling water from 90 °F to 120 °F. This process releases 45 MMBTU/hr of heat. The estimated purchase cost is $123,400 and the installation cost is $391,200.

8.2.7 Reboilers

D-201-R

D-201-R is a kettle reboiler fabricated from carbon steel. It uses steam at 50 psig, at a flow rate of 7,300,000 lbs/hr to heat the boil-up of D-201, which has a flow rate of 93,000 lb/hr. This evaporates the boil-up at 185 °F and condenses the steam. This process transfers 15 MMBTU/hr of heat. The estimated purchase cost is $73,500 and the total bare module cost is $233,000.

D-202-R

D-202-R is a kettle reboiler fabricated from carbon steel. It uses steam at 50 psig, at a flow rate of 3,450,000 lb/hr, to heat the boil-up of D-202, which has a flow rate of 22,000 lb/hr. This evaporates the boil-up at 244 °F and condenses the steam. This process transfers 17 MMBTU/hr of heat. The estimated purchase cost is $59,000 and the total bare module cost is $188,000.

D-203-R

D-203-R is a kettle reboiler fabricated from carbon steel. It uses steam at 50 psig, at a flow rate of 850,000lb/hr, to heat the boil-up of D-203, which has a flow rate of 22,000 lb/hr. This evaporates the boil-up at 244 °F and condenses the steam. This process transfers 17 MMBTU/hr of heat. The estimated purchase cost is $17,800 and the total bare module cost is $56,400.

D-401-R

D-401-R is a kettle reboiler fabricated from stainless steel. It uses steam at 150 psig, at a flow rate of 18,000,000 lb/hr, to heat the boil-up of D-401, which has a flow rate of 22,000 lb/hr. This evaporates the boil-up at 244 °F and condenses the steam. This process transfers 17 MMBTU/hr of heat. The estimated purchase cost is $329,300 and the total bare module cost is $1,043,881.

D-402-R

D-402-R is a kettle reboiler fabricated from stainless steel. It uses steam at 50 psig, at a flow rate of 690,000 lb/hr, to heat the boil-up of D-402, which has a flow rate of 73,600 lb/hr. This evaporates the boil-up at 273 °F and condenses the steam. This process transfers 4.2 MMBTU/hr of heat. The estimated purchase cost is $15,800 and the total bare module cost is $48,190.

D-403-R

D-403-R is a kettle reboiler fabricated from stainless steel. It uses steam at 450 psig, at a flow rate of 143,000 lb/hr, to heat the boil-up of D-403, which has a flow rate of 37,530 lb/hr. This evaporates the boil-up at 425 °F and condenses the steam. This process transfers 7.3 MMBTU/hr of heat. The estimated purchase cost is $60,800 and the total bare module cost is $192,000.

D-404-R

D-404-R is a kettle reboiler fabricated from stainless steel. It uses steam at 450 psig, at a flow rate of 6,600,000 lb/hr, to heat the boil-up of D-404, which has a flow rate of 137,100 lb/hr. This evaporates the boil-up at 503 °F and condenses the steam. This process transfers 40 MMBTU/hr of heat. The estimated purchase cost is $440,900 and the total bare module cost is $1,397,653.

D-405-R

D-405-R is a kettle reboiler fabricated from stainless steel. It uses steam at 450 psig, at a flow rate of 7,900,000 lb/hr, to heat the boil-up of D-405, which has a flow rate of 22,000 lb/hr. This evaporates the boil-up at 244 °F and condenses the steam. This process transfers 17 MMBTU/hr of heat. The estimated purchase cost is $111,600 and the total bare module cost is $354,000.

8.2.8 Reflux Accumulators

D-201-RA

D-201-RA (Figure 200) is a carbon steel horizontal vessel, used as a reflux accumulator for D-201. It has a residence time of 5 min at half capacity. The liquid capacity is 6333 gallons. The estimated purchase cost of RA-201 is $65,300 and the installation cost is $200,000. The reflux accumulator is 7 ft in diameter and 22 ft in length.

D-202-RA

D-202-RA (Figure 200) is a carbon steel horizontal vessel, used as a reflux accumulator for D-202. It has a residence time of 5 min at half capacity. The liquid capacity is 2932 gallons. The estimated purchase cost of RA-202 is $34,500 and the instillation cost is $120,900. The reflux accumulator is 5.5 ft in diameter and 16.5 ft in length.

D-203-RA

D-203-RA (Figure 200) is a carbon steel horizontal vessel, used as a reflux accumulator for D-203. It has a residence time of 5 min at half capacity. The liquid capacity is 719 gallons. The estimated purchase cost of RA-203 is $13,900 and the total purchase and instillation cost is $42,400. The reflux accumulator is 3.5 ft in diameter and 10 ft in length.

D-401-RA

D-401-RA (Figure 400) is a stainless horizontal vessel, used as a reflux accumulator for D-401. It has a residence time of 5 min at half capacity. The liquid capacity is 3022 gallons. The estimated purchase cost of RA-401 is $25,100 and the total purchase and instillation cost is $76,600. The reflux accumulator is 5.5 ft in diameter and 17 ft in length.

D-402-RA

D-402-RA (Figure 400) is a stainless horizontal vessel, used as a reflux accumulator for D-402. It has a residence time of 5 min at half capacity. The liquid capacity is 370 gallons. The estimated purchase cost of RA-402 is $23,900 and the total purchase and installation cost is $72,900. The reflux accumulator is 3 ft in diameter and 7 ft in length.

D-403-RA

D-403-RA (Figure 400) is a stainless horizontal vessel, used as a reflux accumulator for D-403. It has a residence time of 5 min at half capacity. The liquid capacity is 212 gallons. The estimated purchase cost of RA-403 is $13,900 and the total purchase and instillation cost is $42,400. The reflux accumulator is 3 ft in diameter and 4 ft in length.

D-404-RA

D-404-RA (Figure 400) is a stainless horizontal vessel, used as a reflux accumulator for D-404. It has a residence time of 5 min at half capacity. The liquid capacity is 2840 gallons. The estimated purchase cost of RA-404 is $28,500 and the total purchase and instillation cost is $87,000. The reflux accumulator is 5.5ft in diameter and 16 ft in length.

D-405-RA

D-405-RA (Figure 400) is a stainless horizontal vessel, used as a reflux accumulator for D-405. It has a residence time of 5 min at half capacity. The liquid capacity is 3021 gallons. The estimated purchase cost of RA-405 is $23,600 and the total purchase and instillation cost is $72,000. The reflux accumulator is 5.5ft in diameter and 17 ft in length.

8.2.9 Reflux Pumps

D-201-RP

D-201-RP (Figure 200) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-201 tower. The reflux flows at a rate of 11,200 lbmol/hr. The pump has a liquid flow rate of 1043 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $17,200 and the total installation cost is $54,200.

D-202-RP

D-202-RP (Figure 200) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-202 tower. The reflux flows at a rate of 11,200 lbmol/hr. The pump has a liquid flow rate of 443 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $9,300 and the total installation cost is $30,000.

D-203-RP

D-203-RP (Figure 200) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-203 tower. The reflux flows at a rate of 310 lbmol/hr. The pump has a liquid flow rate of 105 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $17,200 and the total installation cost is $54,200.

D-401-RP

D-401-RP (Figure 400) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-401 tower. The reflux flows at a rate of 6437 lbmol/hr. The pump has a liquid flow rate of 504 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $11,400 and the total installation cost is $36,000.

D-402-RP

D-402-RP (Figure 400) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-402 tower. The reflux flows at a rate of 954 lbmol/hr. The pump has a liquid flow rate of 161 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $5,200 and the total installation cost is $17,200.

D-403-RP

D-403-RP (Figure 400) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-403 tower. The reflux flows at a rate of 198 lbmol/hr. The pump has a liquid flow rate of 33 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $11,400 and the total installation cost is $37,620.

D-404-RP

D-404-RP (Figure 400) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-404 tower. The reflux flows at a rate of 2430 lbmol/hr. The pump has a liquid flow rate of 418 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $9,200 and the total installation cost is $30,360.

D-405-RP

D-405-RP (Figure 400) is a cast iron 3600 RPM centrifugal pump, which is used to pump the reflux back to the top of the D-405 tower. The reflux flows at a rate of 2812 lbmol/hr. The pump has a liquid flow rate of 472 gpm and an efficiency of 70%. The estimated purchase cost of P-404 is $10,400 and the total installation cost is $36,630.

8.2.10 Flash Vessels

F-401

The process contains only one flash vessel located in extractive distillation. Before entering the distillation columns, this vessel is used to separate the liquid and vapor phases as well as lower the temperature and pressure to the required amounts for the first distillation column. The flash runs at 100 F and 105 psi. The purchase cost for the vessel is $21,100 and the installed cost is $88,000.

8.2.11 Storage Tanks

T-101

T-101 is a carbon steel, flat bottom API 650 storage tank. It stores the propylene before it is fed into the metathesis process. The tank has a diameter of 66 feet and is 22 feet tall. It has a storage capacity of 2,250,000 gallons, and has a hold-up time of 7 days. It operates at 80 °F and 15 psi. In order to keep the propylene in the liquid phase, nitrogen gas flows through the tank. The purchase cost of T-101 is $700,000 and the total purchase and its bare module cost is $2,100,000.

T-201

T-201 is a carbon steel, pressurized storage tank. It stores the ethylene product formed during distillation so that it can be sold. The tank has a diameter of 12.3 feet and is 49 feet tall. The hold up time is eight hours and it is filled till 70% capacity. The capacity of the tank is 43,250 gallons. It operates at 110 °F and 88 psi. The estimated purchase cost of T- 201 is $61,320 and the bare module cost is $184,000.

T-202

T-202 is a carbon steel, pressurized storage tank. It stores the gasoline product formed during distillation so that it can be sold. The tank has a diameter of 9 feet and is 36 feet tall. The hold up time is 24 hours and it is filled till 70% capacity. The capacity of the tank is 16,920 gallons. It operates at 110 °F and 88 psi. The estimated purchase cost of ST- 401 is $38,000 and the bare module cost is $114,000.

T-401

T-401 is a carbon steel, pressurized storage tank. It stores the 1,3-butadiene product so that it can be sold and its quality. The tank has a diameter of 7 feet and is 30 feet tall. The hold up time is 24 hours and it is filled till 70% capacity. The capacity of the tank is 13,800 gallons. It operates at 110 °F and 88 psi. The purchase cost of is $35,000 and the bare module cost is $105,000.

T-402

T-402 is a carbon steel, pressurized storage tank. It stores the NMP from the purge stream that can be sold for a profit. The NMP is very pure. The tank has a diameter of 4 feet and is 20 feet tall. The holdup time is 24 hours and it is filled till 70% capacity. The capacity of the tank is 960 gallons. It operates at 110 °F and 88 psi. The estimated purchase cost of T-402 is $28,000 and the bare module cost is $84,000.

8.3 Unit Specification Sheets

8.3.1 Pumps

P-201				
Identification	**Equipment**	Pump		
	Inlet Stream	S-202		
	Outlet Stream	S-203		
Function	Pump bottoms product of D-201			
Type	Centrifugal pump 3600 RPM, VSC, 40-500 ft, 40-900 gpm, 75 HP			
Design	**Efficiency** (%)	0.7	**Inlet Pressure** (psia)	404
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	300
	Fluid Head (ft)	-597	**Net Work** (HP)	-20
	Liquid Flow Rate (GPM)	460	**Electricity** (kW)	-14.7
	Installed Weight (lbs)	10607		
Cost	**Purchase** (USD)	8800	**Bare Module** (USD)	29040

P-202				
Identification	**Equipment**		Pump	
	Inlet Stream	S-205		
	Outlet Stream	S-206		
Function	Pump the bottoms product of D-202 to the next distillation column			
Type	Centrifugal pump 3600 RPM, VSC, 40-500 ft, 40-900 gpm, 75 HP			
Design	**Efficiency** (%)	0.54	**Inlet Pressure** (psia)	303
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	103
	Fluid Head (ft)	-1077	**Net Work** (HP)	-6.41
	Liquid Flow Rate (GPM)	102	**Electricity** (kW)	-4.78
	Installed Weight (lbs)	4880		
Cost	**Purchase** (USD)	5800	**Bare Module** (USD)	19140

P-401				
Identification	**Equipment**	Pump		
	Inlet Stream	S-422		
	Outlet Stream	S-423		
Function	Pump Recycle Stream, S-419 into D-402			
Type	Centrifugal pump 3600 RPM, VSC, 40-500 ft, 40-900 gpm, 75 HP			
Design	**Efficiency** (%)	0.57	**Inlet Pressure** (psia)	100
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	501
	Fluid Head (ft)	1215	**Net Work** (HP)	53.5
	Liquid Flow Rate (GPM)	130	**Electricity** (kW)	39.9
	Installed Weight (lbs)	9389		
Cost	**Purchase** (USD)	53500	**Bare Module** (USD)	176550

P-402				
Identification	**Equipment**	Pump		
	Inlet Stream	S-425		
	Outlet Stream	S-426		
Function				
Type	Centrifugal pump 3600 RPM, VSC, 40-500 ft, 40-900 gpm, 75 HP			
Design	**Efficiency** (%)	0.57	**Inlet Pressure** (psia)	100
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	501
	Fluid Head (ft)	1215	**Net Work** (HP)	53.5
	Liquid Flow Rate (GPM)	130	**Electricity** (kW)	40
	Installed Weight (lbs)			
Cost	**Purchase** (USD)	53500	**Bare Module** (USD)	176550

P-403				
Identification	**Equipment**	Pump		
	Inlet Stream	S-427		
	Outlet Stream	S-428		
Function	Pump Recycle Stream, S-416 into D-403			
Type	Centrifugal pump 3600 RPM, VSC, 40-500 ft, 40-900 gpm, 75 HP			
Design	**Efficiency** (%)	0.5	**Inlet Pressure** (psia)	14.7
	Casing Material	Cast Iron	**Outlet Pressure** (psia)	201
	Fluid Head (ft)	436	**Net Work** (HP)	16.8
	Liquid Flow Rate (GPM)	77.3	**Electricity** (kW)	12.5
	Installed Weight (lbs)	9295		
Cost	**Purchase** (USD)	53500	**Bare Module** (USD)	176550

8.3.2 Heat Exchangers

H-101				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S-103	**Inlet Cold Temperature** (F)	114.7
	Outlet Stream	S-104	**Outlet Cold Temperature** (F)	302
Function	Heat feed stream into metathesis process and cool S-114 before distillation			
Type	Shell and Tube			
Design	**Exchange Area** (ft2)	545	**Installed Weight** (lbs)	
	Tube Temperature (F)	574	**Tube Material**	Stainless Steel
	Shell Temperature (F)	574	**Shell Material**	Carbon Steel
	Tube Pitch (in)	1.25	**Tube Length**	20
Cost	**Purchase** (USD)	12005	**Bare Module** (USD)	70341

H-301				
Identification	**Equipment**	Heat Exchanger		
	Inlet Stream	S-303	**Inlet Temperature** (F)	371.9
	Outlet Stream	S-304	**Outlet Temperature** (F)	752
Function	Heat air feed into Oxidative Dehydrogenation Reactor			
Type	Shell and Tube			
Design	**Exchange Area** (ft2)	89.6	**Installed Weight** (lbs)	
	Tube Temperature (F)		**Tube Material**	Stainless Steel
	Shell Temperature (F)	100	**Shell Material**	Carbon Steel
	Tube Pitch (in)	1.25	**Tube Length**	20
Cost	**Purchase** (USD)	11300	**Bare Module** (USD)	35984

H-302				
Identification	**Equipment**	Heat Exchanger		
	Inlet Cold Stream	S-208	**Cold Inlet Temperature** (F)	143
	Outlet Cold Stream	S-308	**Cold Outlet Temperature** (F)	449
	Inlet Hot Stream	S-307	**Hot Inlet Temperature** (F)	752
	Outlet Hot Stream	S-301	**Hot Outlet Temperature** (F)	485
Function	Heat Distillation effluent into Oxy-D reactor by using heat from reactor effluent			
Type	Shell and Tube			
Design	**Exchange Area** (ft2)	100	**Installed Weight** (lbs)	10847
	Tube Temperature (F)	802	**Tube Material**	Stainless Steel
	Shell Temperature (F)	802	**Shell Material**	Carbon Steel
	Tube Pitch (in)	1.25	**Tube Length**	20
Cost	**Purchase** (USD)	11200	**Bare Module** (USD)	35504

8.3.3 Flash Vessel

F-101				
Identification	**Equipment**	Flash Vessel		
	Inlet Stream	S-401		
	Overhead	S-402		
	Bottoms	S-403		
Function	Flash stream to a lower temp and pressure to prepare for extractive distillaton			
Design	**Temperature** (F)	100	**Construction Material**	Low-Alloy Steel
	Pressure (psia)	105	**Vessel Wall Thickness** (in)	0.15
	Bottoms Flow Rate (lb/hr)	7307	**Installed Weight** (lbs)	19030
	Vapor Flow Rate	44860	**Diameter** (ft)	3.5
	Liquid Volume (Gal)	863	**Vessel Tangent Height** (ft)	12
Cost	**Purchase** (USD)	17,900	**Bare Module** (USD)	104,300

8.3.4 Distillation Columns

D-201				
Identification	**Equipment**	Distillation Column		
Function	Separate ethylene from Metathesis Effluent			
Design	**Number of Trays**	20	**Tray Spacing** (ft)	2
	Total Weight (lbs)	287130	**Tray Type**	Sieve
	Feed Stage	10	**Tray Efficiency** (%)	0.7
	Total Height (ft)	63	**Condenser Type**	Total
	Construction Material	Carbon Steel	**Condenser Duty** (Btu/hr)	-3.93E+7
	Reboiler Pressure (psia)	404	**Reboiler Duty (Btu/hr)**	3.65E+7
	Condenser Pressure (psia)	400	**Reflux Ratio**	26.7
	Column Diameter (ft)	10.5		
Materials	**Feed**	**Liquid Distillate**	**Bottoms**	**--**
Stream ID	S-112	S-202	S-201	
Temperature (F)	160	2.3	185.3	
Pressure (psia)	400	400	403.98	
Total Flow Rate (lb/hr)	104300	11750	92500	
Component Flow Rates (lb/hr)				
Propyelene	53300	176	53140	
Ethylene	11600	11580	11.6	
Trans-2-Butene	20230		20230	
Cis-2-Butene	12400		12400	
1-Butene	3690		3700	
Trans-3-Hexene	96.4		96.4	
Cis-2-Pentene	738.964		738.964	
Trans-2-Pentene	2137.039		2137.039	
Cost	**Purchase** (USD)	495,600	**Bare Module** (USD)	2,061,700

D-202				
Identification	**Equipment**	Distillation Column		
Function	Separate propylene for recycle back to metathesis			
Design	**Number of Trays**	10	**Tray Spacing** (ft)	2
	Total Weight (lbs)	63900	**Tray Type**	Sieve
	Feed Stage	5	**Tray Efficiency** (%)	0.7
	Total Height (ft)	35	**Condenser Type**	Total
	Construction Material	Carbon Steel	**Condenser Duty** (Btu/h)	1.8E+7
	Reboiler Pressure (psia)	303	**Reboiler Duty** (Btu/hr)	1.72E+7
	Condenser Pressure (psi)	300	**Reflux Ratio**	1.057
	Column Diameter (ft)	7		

Materials	Feed	Liquid Distillate	Bottoms	--
Stream ID	S-203	S-204	S-205	
Temperature (F)	182.5	139.3	244	
Pressure (psia)	300	300	302.88	
Total Flow Rate (lb/hr)	9.25E+04	7.06E+04	2.19E+04	
Component Flow Rates (lb/hr)				
Propyelene	53180	52600	531.4	
Ethylene	84.5	84.5	0.002	
Trans-2-Butene	20100	10000	10100	
Cis-2-Butene	12400	5240	7130	
1-Butene	3700	2420	1250	
Cis-3-Hexene	22.6	0.047	22.5	
Trans-3-Hexene	95	0.197	94.8	
Cis-2-Pentene	730	23.6	708.8	
Trans-2-Pentene	2120	71.58	2050	
Cost	**Purchase** (USD)	149,900	**Bare Module** (USD)	623,584

D-203				
Identification	**Equipment**	Distillation Column		
Function	Separate Butenes from side products in preparation for metathesis			
Design	**Number of Trays**	10	**Tray Spacing** (ft)	2
	Total Weight (lbs)	27500	**Tray Type**	Sieve
	Feed Stage	5	**Tray Efficiency** (%)	0.7
	Total Height (ft)	35	**Condenser Type**	Total
	Construction Material	Carbon Steel	**Condenser Duty** (Btu/hr)	5.68E+6
	Reboiler Pressure (psia)	102.88	**Reboiler Duty** (Btu/hr)	4.26E+6
	Condenser Pressure (psia)	100	**Reflux Ratio**	0.88
	Column Diameter (ft)	3		

Materials	Feed	Liquid Distillate	Bottoms	--
Stream ID	S-207	S-208	S-209	
Temperature (F)	239.3	217.3	142.8	
Pressure (psia)	103	102.88	100	
Total Flow Rate (lb/hr)	21900	2220	19700	
Component Flow Rates (lb/hr)				
Propyelene	531	.006	535	
Ethylene	0.002		0.015	
Trans-2-Butene	10100	87.4	10020	
Cis-2-Butene	7130	97.6	7030	

1-Butene	1250	4.0	1245	
Cis-3-Hexene	22.5	22.3	0.24	
Trans-3-Hexene	94.8	93.9	0.92	
Cis-2-Pentene	710	500	208	
Trans-2-Pentene	2050	1410	633	
Cost	**Purchase** (USD)	118800	**Bare Module** (USD)	494200

D-401				
Identification	**Equipment**	Distillation Column		
Function	Decant Water formed from Oxidative Dehydrogenation			
Design	**Number of Trays**	10	**Column Diameter** (ft)	8
	Total Weight (lbs)	86300	**Tray Spacing** (ft)	2
	Liquid Feed Stage	8	**Tray Type**	Sieve
	Vapor Feed Stage	3	**Tray Efficiency** (%)	0.7
	Total Height (ft)	35	**Condenser Type**	Par-Vapor
	Construction Material	Low Alloy Steel	**Condenser Duty** (Btu/hr)	-7.54E+7
	Reboiler Pressure (psia)	103.88	**Reboiler Duty** (Btu/hr)	7.65E+7
	Condenser Pressure	101	**Reflux Ratio**	5
Materials	**Liquid Feed**	**Vapor Feed**	**Vapor Distillate**	**Bottoms**
Stream ID	S-403	S-402	S-404	S-405
Temperature (F)	100	100	63.5	330.7
Pressure (psia)	105	105	101	103.88
Total Flow Rate (lb/hr)	14325.28	37847.613	45879.465	6293.427
Component Flow Rates (lb/hr)				
Propyelene	63.7	472	535	0.006
Ethylene		0.015	0.015	
1-Butene	406.5	840	1245	0.178
1-3 Butadiene	58.6	15600	15600	
Carbon Dioxide	65.2	2610	2675	
Oxygen	0.065	27.3	27.3	
Nitrogen	48.6	24870	24920	
Water	6101	197	11.4	6290
Cis-3-Hexene	0.214	0.026	0.089	0.151
Trans-3-Hexene	0.852	0.098	0.342	0.608
Cis-2-Pentene	140	53.446	212.513	0.459
Trans-2-Pentene	422	165	647	1.24
Cost	**Purchase** (USD)	136,800	**Bare Module** (USD)	569,100

D-402				
Identification	**Equipment**	Distillation Column		
Function	Separate vapors formed from oxidative dehydrogenation			
Design	**Number of Trays**	15	**Column Diameter** (ft)	4
	Total Weight (lbs)	63500	**Tray Spacing** (ft)	2
	Liquid Feed Stage	15	**Tray Type**	Sieve
	Vapor Feed Stage	2	**Tray Efficiency** (%)	0.7
	Total Height (ft)	41	**Condenser Type**	Par-Vapor
	Construction Material	Low Alloy Steel	**Condenser Duty** (Btu/hr)	-1.36E+7
	Reboiler Pressure (psia)	503.4	**Reboiler Duty** (Btu/hr)	3.44E+6
	Condenser Pressure (psia)	500	**Reflux Ratio**	1
Materials	**Extractant Feed**	**Feed**	**Vapor Distillate**	**Bottoms**
Stream ID	S-423	S-406	S-407	S-408
Temperature (F)	506.5	317.6	-20.9	269.3
Pressure (psia)	501	501	500	503.4
Total Flow Rate (lb/hr)	49600	45900	27900	67500
Component Flow Rates (lb/hr)				
Propyelene	--	531.3	370.7	160.6
1-Butene	7.08	1245	0.25	1250
1-3 Butadiene	6.43	15600	337.1	15300
Carbon Dioxide	--	2675	2540	138
Oxygen	--	30.6	30.3	0.35
Nitrogen	--	24900	24700	261
Water	0.72	6.34	--	7.05
Cis-3-Hexene	--	0.09	--	0.09
Trans-3-Hexene	--	0.34	--	0.35
Cis-2-Pentene	1.89	212	--	214
Trans-2-Pentene	5.65	646	--	652
NMP	49500		--	49500
Cost	**Purchase** (USD)	118,800	**Bare Module** (USD)	494,200

D-403				
Identification	**Equipment**	Distillation Column		
Function	Separate propylene from C4 products			
Design	**Number of Trays**	20	**Column Diameter** (ft)	4.5
	Total Weight (lbs)	99650	**Tray Spacing** (ft)	2
	Liquid Feed Stage	15	**Tray Type**	Sieve
	Vapor Feed Stage	2	**Tray Efficiency** (%)	0.7
	Total Height (ft)	63	**Condenser Type**	Partial-Vapor-Liquid

	Construction Material	Stainless Steel	**Condenser Duty** (Btu/hr)		-2.47E+06
	Reboiler Pressure (psia)	504	**Reboiler Duty** (Btu/hr)		7.13E+06
	Condenser Pressure (psia)	500	**Reflux Ratio**		5
Materials	**Extractant Feed**	**Feed**	**Vapor Distillate**	**Liquid Distillate**	**Bottoms**
Stream ID	S-426	S-408	S-409	S-410	S-412
Temperature (F)	506.5	269.3	226.8	226.8	426
Pressure (psia)	501	503	500	500	504
Total Flow Rate (lb/hr)	49600	67500	1410	435	115200
Component Flow Rates (lb/hr)					
Propyelene	--	160.6	105	15.8	39.9
1-Butene	7.08	1250	1.82	0.79	1260
1-3 Butadiene	6.43	15300	907	383	14000
Carbon Dioxide	--	138	134	4.20	--
Oxygen	--	0.35	0.35	--	--
Nitrogen	--	262	260.20	1.41	--
Water	0.72	7.05	--	--	7.76
Cis-3-Hexene	--	0.09	--	--	0.09
Trans-3-Hexene	--	0.35	--	--	0.35
Cis-2-Pentene	1.89	214	0.03	0.05	216
Trans-2-Pentene	5.65	652	0.11	0.14	657
NMP	49500	49530	0.37	29.4	99000
Cost	**Purchase** (USD)	173,700	**Bare Module** (USD)		772,600

D-404				
Identification	**Equipment**	Distillation Column		
Function	Separates 1,3 butadiene product using NMP extractant			
Design	**Number of Trays**	35	**Column Diameter** (ft)	6.5
	Total Weight (lbs)	176587	**Tray Spacing** (ft)	2
	Liquid Feed Stage	20	**Tray Type**	Sieve
	Vapor Feed Stage	2	**Tray Efficiency** (%)	0.7
	Total Height (ft)	96	**Condenser Type**	Total
	Construction Material	Stainless Steel	**Condenser Duty** (Btu/hr)	-1.93E+07
	Reboiler Pressure (psia)	205.63	**Reboiler Duty** (Btu/hr)	3.31E+07
	Condenser Pressure (psia)	200	**Reflux Ratio**	10
Materials	**Extractant Feed**	**Feed**	**Liquid Distillate**	**Bottoms**
Stream ID	S-428	S-413	S-414	S-415
Temperature (F)	101.3	442	190.7	556
Pressure (psia)	201	205	200	206
Total Flow Rate (lb/hr)	38200	115200	13100	140200

Component Flow Rates (lb/hr)				
Propyelene	--	40	39.9	--
1-Butene	--	1256	42.6	1210
1-3 Butadiene	--	14000	13050	945
Water	--	7.76	--	7.76
Cis-3-Hexene	--	0.09	--	0.09
Trans-3-Hexene	--	0.35	--	0.35
Cis-2-Pentene	--	216	--	216
Trans-2-Pentene	--	658	--	658
NMP	38200	99000	10.37	137000
Cost	**Purchase** (USD)	331,700	**Bare Module** (USD)	1,138,000

D-405				
Identification	**Equipment**	Distillation Column		
Function	Separate NMP to recycle			
Design	**Number of Trays**	5	**Tray Spacing** (ft)	2
	Total Weight (lbs)	80800	**Tray Type**	Sieve
	Feed Stage	5	**Tray Efficiency** (%)	0.7
	Total Height (ft)	21	**Condenser Type**	Total
	Construction Material	Stainless Steel	**Condenser Duty** (Btu/hr)	-4.58E+7
	Reboiler Pressure (psia)	52.3	**Reboiler Duty** (Btu/hr)	3.95E+7
	Condenser Pressure (psia)	50	**Reflux Ratio**	50.7
	Column Diameter (ft)	9.5		
Materials	**Feed**	**Liquid Distillate**	**Bottoms**	**--**
Stream ID	S-415	S-416	S-417	
Temperature (F)	556	105	504	
Pressure (psia)	206	50	52	
Total Flow Rate (lb/hr)	140200	3430	136800	
Component Flow Rates (lb/hr)				
1-Butene	1210	1200	19.6	
1-3 Butadiene	945	927	17.8	
Water	7.76	5.78	1.98	
Cis-3-Hexene	0.09	0.09		
Trans-3-Hexene	0.35	0.34	0.01	
Cis-2-Pentene	216	211	5.23	
Trans-2-Pentene	657	642	15.65	
NMP	137000	448	137000	
Cost	**Purchase** (USD)	103,200	**Bare Module** (USD)	429,300

8.3.5 Reactors

R-101				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-108		
	Outlet Stream	S-114		
Main Reactions	2 Propylene --> Ethylene + Cis-2-Butene			
	2 Propylene --> Ethylene + Trans-2-Butene			
Side Reactions	Cis-2-Butene --> 1-Butene			
	Trans-2-Butene --> 1-Butene			
	1-Butene + Propylene --> Ethylene + Cis-2-Pentene			
	1-Butene + Propylene --> Ethylene + Trans-2-Pentene			
	2 1-Butene --> Ethylene + Cis-3-Hexene			
	2 1-Butene --> Ethylene + Trans-3-Hexene			
Classification	Shell and Tube, Packed Bed			
Design	**Temperature** (F)	302	**Volume** (gal)	122300
	Pressure (psia)	29.39	**Construction Material**	Carbon Steel
	Diameter (ft)	20	**Heat Duty** (Btu/hr)	1767003
	Height (ft)	66	**Residence Time** (hr)	0.05
	Electricity (kW)		**Vessel Weight** (lbs)	64328
Component Flow Rates (lb/hr)				
	Inlet		**Outlet**	
Propyelene		43135.28		27489.97
Ethylene		5.80		5220.90
Trans-2-Butene		5066.25		11241.53
Cis-2-Butene		2652.70		6907.63
1-Butene		1221.52		1221.52
Cis-3-Hexene		0.03		0.03
Trans-3-Hexene		0.10		0.10
Cis-2-Pentene		12.12		12.12
Trans-2-Pentene		36.65		36.65
Cost	**Purchase** (USD)	504,904	**Bare Module** (USD)	852,400.90
	Cost of Catalyst (USD)	$52,130	**Total Bare Module** (USD)	$904,530.90

R-102		
Identification	**Equipment**	Reactor
	Inlet Stream	S-109
	Outlet Stream	S-115
Main Reactions	2 Propylene --> Ethylene + Cis-2-Butene	
	2 Propylene --> Ethylene + Trans-2-Butene	

Side Reactions	Cis-2-Butene --> 1-Butene Trans-2-Butene --> 1-Butene 1-Butene + Propylene --> Ethylene + Cis-2-Pentene 1-Butene + Propylene --> Ethylene + Trans-2-Pentene 2 1-Butene --> Ethylene + Cis-3-Hexene 2 1-Butene --> Ethylene + Trans-3-Hexene			
Classification	Shell and Tube, Packed Bed			
Design	**Temperature** (F)	302	**Volume** (gal)	122300
	Pressure (psia)	29.39	**Construction Material**	Carbon Steel
	Diameter (ft)	20	**Heat Duty** (Btu/hr)	1767003
	Height (ft)	66	**Residence Time** (hr)	0.05
	Electricity (kW)		**Vessel Weight** (lbs)	64328
Component Flow Rates (lb/hr)				
	Inlet		**Outlet**	
Propyelene		43135.28		27489.97
Ethylene		5.80		5220.90
Trans-2-Butene		5066.25		11241.53
Cis-2-Butene		2652.70		6907.63
1-Butene		1221.52		1221.52
Cis-3-Hexene		0.03		0.03
Trans-3-Hexene		0.10		0.10
Cis-2-Pentene		12.12		12.12
Trans-2-Pentene		36.65		36.65
Cost	**Purchase** (USD)	504,904	**Bare Module** (USD)	852,400.90
	Cost of Catalyst (USD)	$52,130	**Total Bare Module** (USD)	$904,530.90

R-103		
Identification	**Equipment**	Reactor
	Inlet Stream	S-111
	Outlet Stream	S-116
Main Reactions	2 Propylene --> Ethylene + Cis-2-Butene 2 Propylene --> Ethylene + Trans-2-Butene	
Side Reactions	Cis-2-Butene --> 1-Butene Trans-2-Butene --> 1-Butene 1-Butene + Propylene --> Ethylene + Cis-2-Pentene 1-Butene + Propylene --> Ethylene + Trans-2-Pentene 2 1-Butene --> Ethylene + Cis-3-Hexene 2 1-Butene --> Ethylene + Trans-3-Hexene	
Classification	Shell and Tube, Packed Bed	

Design	**Temperature** (F)	302	**Volume** (gal)	122300
	Pressure (psia)	29.39	**Construction Material**	Carbon Steel
	Diameter (ft)	20	**Heat Duty** (Btu/hr)	1767003
	Height (ft)	66	**Residence Time** (hr)	0.05
	Electricity (kW)		**Vessel Weight** (lbs)	64328
Component Flow Rates (lb/hr)				
	Inlet		**Outlet**	
Propyelene		43135.28		27489.97
Ethylene		5.80		5220.90
Trans-2-Butene		5066.25		11241.53
Cis-2-Butene		2652.70		6907.63
1-Butene		1221.52		1221.52
Cis-3-Hexene		0.03		0.03
Trans-3-Hexene		0.10		0.10
Cis-2-Pentene		12.12		12.12
Trans-2-Pentene		36.65		36.65
Cost	**Purchase** (USD)	504,904	**Bare Module** (USD)	852,400.90
	Cost of Catalyst (USD)	$52,130	**Total Bare Module** (USD)	$904,530.90

R-301				
Identification	**Equipment**	Reactor		
	Inlet Stream	S-303, Air S-306		
	Outlet Stream	S-307		
Main Reactions	Cis-2-Butene + 1/2 Oxygen --> 1,3 Butadiene + Water			
	Trans-2-Butene + 1/2 Oxygen --> 1,3 Butadiene + Water			
Side Reactions	Cis-2-Butene + 6 Oxygen --> 4 Carbon Dioxide + 4 Water			
	Trans-2-Butene + 6 Oxygen --> 4 Carbon Dioxide + 4 Water			
Classification	Shell and Tube, Packed Bed			
Design	**Temperature** (F)	752	**Volume** (gal)	
	Pressure (psia)	44	**Construction Material**	Carbon Steel
	Diameter (ft)		**Heat Duty** (Btu/hr)	-31100000
	Height (ft)		**Residence Time** (hr)	
	Electricity (kW)	--	**Vessel Weight** (lbs)	
Component Flow Rates (lb/hr)				
	Inlet Feed	**Inlet Air**	**Outlet**	
Propyelene	535		532	
Ethylene	0.015		0.002	
Trans-2-Butene	10025			
Cis-2-Butene	7032			
1-Butene	1250		1250	
1-3 Butadiene			15620	

Carbon Dioxide				2675
Oxygen		7570		31
Nitrogen		24920		24920
Water				6300
Cis-3-Hexene	0.233			0.24
Trans-3-Hexene	0.924			0.95
Cis-2-Pentene	208			213
Trans-2-Pentene	633			648
Cost	**Purchase** (USD)	$504,900	**Bare Module** (USD)	$852,400.00
	Cost of Catalyst (USD)	$52,130	**Total Bare Module** (USD)	$904,530.00

8.3.6 Compressors

C-101				
Identification	**Equipment**	Compressor		
Function	Pressurize effluent of metathesis reactors in preparation for distillation			
Classification	Centrifugal Isentropic			
Design	**Gas Flow Inlet** (CFM)	10873.25	**Construction Material**	Carbon Steel
	Inlet Pressure (psia)	29.39	**Outlet Pressure** (psia)	400
	Motor Power (HP)	5394	**Installed Weight** (lbs)	21183
Cost	**Purchase** (USD)	$2,478,100	**Bare Module** (USD)	$5,327,915

C-301				
Identification	**Equipment**	Compressor		
Function	Pressurize air feed for oxidative dehydrogenation			
Classification	Centrifugal Isentropic			
Design	**Gas Flow Inlet** (CFM)	7234.22	**Construction Material**	Carbon Steel
	Inlet Pressure (psia)	14.7	**Outlet Pressure** (psia)	50
	Motor Power (HP)	944	**Installed Weight** (lbs)	52000
Cost	**Purchase** (USD)	$1,236,000	**Bare Module** (USD)	$2,657,830

C-401				
Identification	**Equipment**	Compressor		
Function	Stabilize pressure of vapor distillate of D-401 in preparation for D-402			
Classification	Centrifugal Isentropic			
Design	**Gas Flow Inlet** (CFM)	1192.64	**Construction Material**	Carbon Steel
	Inlet Pressure (psia)	101	**Outlet Pressure** (psia)	501
	Motor Power (HP)	1362	**Installed Weight** (lbs)	49000
Cost	**Purchase** (USD)	$1,257,000	**Bare Module** (USD)	$2,704,055

8.3.7 Storage Tanks

T-101				
Identification	Storage Tank			
Function	Store Propylene Feed			
Classification	Carbon Steel Flat Bottom			
Design	**Capacity (gal)**	2,250,000	**Residence Time**	7 days
	Pressure (psia)	88	**Diameter (ft)**	66
	Temperature (F)	110	**Height (ft)**	22
Cost	**Purchase** (USD)	$700,000	**Bare Module** (USD)	$2,100,000
T-201				
Identification	Storage Tank			
Function	Store Ethylene as it forms in Distillation			
Classification	Carbon Steel Flat Bottom			
Design	**Capacity (gal)**	43,250	**Residence Time**	8 hours
	Pressure (psia)	88	**Diameter (ft)**	12.3
	Temperature (F)	110	**Height (ft)**	49
Cost	**Purchase** (USD)	$61,320	**Bare Module** (USD)	$183,960

T-202				
Identification	Storage Tank			
Function	Store Gasoline by product			
Classification	Carbon Steel Flat Bottom			
Design	**Capacity (gal)**	16,920	**Residence Time**	1 day
	Pressure (psia)	88	**Diameter (ft)**	9
	Temperature (F)	110	**Height (ft)**	36
Cost	**Purchase** (USD)	$38,000	**Bare Module** (USD)	$114,000

T-401				
Identification	Storage Tank			
Function	Store 1,3 Butadiene			
Classification	Carbon Steel Flat Bottom			
Design	**Capacity (gal)**	13,800	**Residence Time**	1 day
	Pressure (psia)	88	**Diameter (ft)**	7
	Temperature (F)	110	**Height (ft)**	30
Cost	**Purchase** (USD)	$35,000	**Bare Module** (USD)	$105,000

T-402				
Identification	Storage Tank			
Function	Store NMP from the purge			
Classification	Carbon Steel Flat Bottom			
Design	**Capacity (gal)**	960	**Residence Time**	1 day
	Pressure (psia)	88	**Diameter (ft)**	4
	Temperature (F)	110	**Height (ft)**	20
Cost	**Purchase** (USD)	$28,000	**Bare Module** (USD)	$84,000

9.0 COSTING

9.1 EQUIPMENT COSTING

The below shows the purchase and bare module cost of all the equipment modeled on our Aspen Flow Sheet. All costing was one using ASPEN IPE except for Reactors and one heat exchanger. Reactors were sized using calculations in Seider et al and are shown in the Appendix.

Equipment Description	Type	Purchase Cost	Bare Module Cost
P-201 centrifugal pump	Process Machinery	$8,800	$29,040
P-202 centrifugal pump	Process Machinery	$5,800	$19,140
P-401 centrifugal pump	Process Machinery	$53,500	$176,550
P-402 centrifugal pump	Process Machinery	$53,500	$176,550
P-403 centrifugal pump	Process Machinery	$17,200	$56,760
C-101 compressor	Process Machinery	$2,478,100	$5,327,915
C-301 compressor	Process Machinery	$1,236,200	$2,657,830
C-401 compressor	Process Machinery	$1,257,700	$2,704,055
D-201 condenser	Fabricated Equipment	$2,952,000	$12,280,320
D-201 reflux accumulator	Fabricated Equipment	$65,300	$199,165
D-201 reboiler	Fabricated Equipment	$73,500	$232,995
D-201 reflux pump	Fabricated Equipment	$17,200	$56,760
D-201 tower	Fabricated Equipment	$495,600	$2,061,696
D-202 condenser	Fabricated Equipment	$86,400	$359,424
D-202 reflux accumulator	Fabricated Equipment	$34,500	$105,225
D-202 reboiler	Fabricated Equipment	$59,300	$187,981
D-202 reflux pump	Fabricated Equipment	$9,300	$30,690
D-202 tower	Fabricated Equipment	$149,900	$623,584
D-203 condenser	Fabricated Equipment	$28,100	$116,896
D-203 reflux accumulator	Fabricated Equipment	$13,900	$42,395
D-203 reboiler	Fabricated Equipment	$17,800	$56,426
D-203 reflux pump	Fabricated Equipment	$17,200	$56,760
D-203 tower	Fabricated Equipment	$118,000	$490,880
D-401 condenser	Fabricated Equipment	$28,100	$116,896
D-401 reflux accumulator	Fabricated Equipment	$25,100	$76,555
D-401 reboiler	Fabricated Equipment	$329,300	$1,043,881
D-401 reflux pump	Fabricated Equipment	$11,400	$37,620
D-401 tower	Fabricated Equipment	$136,800	$569,088

D-402 condenser	Fabricated Equipment	$281,500	$1,171,040
D-402 reflux accumulator	Fabricated Equipment	$23,900	$72,895
D-402 reboiler	Fabricated Equipment	$15,800	$50,086
D-402 reflux pump	Fabricated Equipment	$5,200	$17,160
D-402 tower	Fabricated Equipment	$118,800	$494,208
D-403 condenser	Fabricated Equipment	$9,900	$41,184
D-403 reflux accumulator	Fabricated Equipment	$13,900	$42,395
D-403 reboiler	Fabricated Equipment	$60,800	$192,736
D-403 reflux pump	Fabricated Equipment	$11,400	$37,620
20D-403 tower	Fabricated Equipment	$210,700	$876,512
D-404 condenser	Fabricated Equipment	$40,200	$167,232
D-404 reflux accumulator	Fabricated Equipment	$28,500	$86,925
D-404 reboiler	Fabricated Equipment	$440,900	$1,397,653
D-404 reflux pump	Fabricated Equipment	$9,200	$30,360
D-404 tower	Fabricated Equipment	$331,700	$1,379,872
D-405 condenser	Fabricated Equipment	$123,400	$513,344
D-405 reflux accumulator	Fabricated Equipment	$23,600	$71,980
D-405 reboiler	Fabricated Equipment	$111,600	$353,772
D-405 reflux pump	Fabricated Equipment	$10,400	$34,320
D-405 tower	Fabricated Equipment	$103,200	$429,312
F-401 flash vessel	Fabricated Equipment	$21,100	$87,776
H-101 shell & tube heat exchanger	Fabricated Equipment	$14,000	$44,380
H-301 shell & tube heat exchanger	Fabricated Equipment	$11,340	$35,948
H-302 shell &-tube heat exchanger	Fabricated Equipment	$16,040	$50,847
H-303 shell & tube heat exchanger	Fabricated Equipment	$15,200	$48,184
R-101 reactor	Fabricated Equipment	$296,900	$1,276,670
R-102 reactor	Fabricated Equipment	$296,900	$1,276,670
R-103 reactor	Fabricated Equipment	$296,900	$1,276,670
R-301 reactor	Fabricated Equipment	$38,000	$881,087
T-101 Storage Tank	Fabricated Equipment	$700,000	$2,100,000
T-201 Storage Tank	Fabricated Equipment	$61,320	$184,000
T-202 Storage Tank	Fabricated Equipment	$38,000	$114,000
T-401 Storage Tank	Fabricated Equipment	$35,000	$105,000

T-402 Storage Tank	Fabricated Equipment	$28,000	$84,000
Total Cost		**$13,769,550**	**$44,918,915**

9.2 Operating Costs

The economic analysis is based on the results generated by Profitability Analysis Spreadsheet 4.0 provided by Seider et al. The costs can be divided between total capital investment needed ensure production and the continuous operation of the manufacturing plant.

9.2.1 Fixed Capital Investment

Capital Investment	Price
Total Bare Module Cost for Equipment	$33,497,432
Total Bare Module Costs for Spare	N/A
Total Bare Module Costs for Storage Tanks	$900,000
Total Cost on Catalysts	$24,500
Total Bare Module Investment, TBM	$34,421,932
Cost of Site Preparation	$390,120
Cost of Services Facilities	$260,008
Utility Plants And Related Facilities	
Direct Permanent Investment	$3,251,000
Total Depreciable Capital	$3,836,100
Cost of Land	$67,517
Cost of Royalties	N/A
Cost of Plant Start Up	$337,584
Total Permanent Investment, TPI	$4,297,000
Total Capital Investment, TCI	**$17,944,000**

Assumptions that were made in the above costing of Total Capital Investment include that the cost of site preparation was set at 15% since it is a grass-roots plant. The cost of service facilities was set at 10% because there is high utility usage associated with this design.

9.2.2 Working Capital

The working capital is needed to cover early operational costs for the plant. The Working Inventory computed below is based on a 4 day 1,3-butadiene and a 2 –day raw material Inventory. It also assumes an 30 day accounts receivable, payable and cash reserve.

	2018	2019	2020
Accounts Receivable	$4,109,589	$2,054,795	$2,054,795
Cash Reserves	$72,345	$36,173	$36,173
Accounts Payable	$(25,059,041)	$(12,529,521)	$(12,529,521)
1,3-Butadiene	$547,945	$273,973	$273,973
Raw Materials	$1,670,603	$835,301	$835,301
Total	**$(18,658,559)**	**$(9,329,279)**	**$(9,329,279)**

9.2.3 Variable Cost Summary

The variable cost summary includes General Expenses, Raw Materials and Utilities with a subtraction of the profits made from selling byproducts of the process. The General Expenses include Selling and Transfer Expenses (3%), Allocated Research (0.5%), administrative expenses (2%) and Management incentive Compensation (1.25%) of Sales. Since the Metathesis process has a catalyst that has not yet been developed, 7% of Sales will be allocated towards Direct Research.

The by-products are Ethylene, Gasoline, and NMP from the 1% purge out of extractive distillation that are sold at $0.12/lb, $0.65/lb and $1.25/lb respectively. The breakdown of the utilities is present in section 7.2.

General Expenses	Selling / Transfer Expenses:		$3,000,000
	Direct Research:		$7,000,000
	Allocated Research:		$500,000
	Administrative Expense:		$2,000,000
	Management Incentive Compensation:		$1,250,000
Total General Expenses			$13,750,000
Raw Materials	$6.097700	per lb of 1,3-Butadiene	$609,770,000
Byproducts	$4.225620	per lb of 1,3-Butadiene	($422,562,000)
Utilities	$0.000000	per lb of 1,3-Butadiene	$0
Total Variable Costs			**$200,958,000**

9.2.4 *Fixed Cost Summary*

The fixed cost is the sum of the total cost of operations, maintenance, operating overhead, property taxes and insurance and other annual expenses. It is $1.7 Million for this plant.

Operations	
Direct Wages and Benefits	$416,000
Direct Salaries and Benefits	$62,400
Operating Supplies and Services	$24,960
Technical Assistance to Manufacturing	$300,000
Control Laboratory	$325,000
Total Operations	$1,128,360
Maintenance	
Wages and Benefits	$172,628
Salaries and Benefits	$43,157
Materials and Services	$172,628
Maintenance Overhead	$8,631
Total Maintenance	$397,045
Operating Overhead	
General Plant Overhead:	$49,287
Mechanical Department Services:	$16,660
Employee Relations Department:	$40,957
Business Services:	$51,370
Total Operating Overhead	$158,274
Property Taxes and Insurance	
Property Taxes and Insurance:	$76,724
Other Annual Expenses	
Rental Fees (Office and Laboratory Space):	$-
Licensing Fees:	$-
Miscellaneous:	$-
Total Other Annual Expenses	$-
Total Fixed Costs	**$1,760,402**

9.3 Economic Analysis

We are making a significantly high negative ROI of 202%. This is largest attributable to the high cost of raw materials. Its costs $1.89 of raw materials to produce $1 of our product, 1,3-butadiene. This is primarily due to the 2:1 stoichiometric ratio of propylene to butene in the metathesis reaction. Because propylene cost is $0.65/lb and 1,3-butadiene sells for only $1.00/lb, this immediately puts our losses at $0.30/lb of 1,3-butadiene. While selling our byproducts of gasoline hydrocarbons and ethylene helps reduce this loss, it is not enough to make the process profitable considering the additional costs of utilities and capital.

ROI Analysis (Third Production Year)	
Annual Sales	103,225,600
Annual Costs	(209,257,287)
Depreciation	(343,722)
Income Tax	39,358,901
Net Earnings	(67,016,508)
Total Capital Investment	(33,020,596)
ROI	**202.95%**

While our process may not be profitable at current prices of 1,3-butadiene and propylene, if market trends go as predicted and the movement toward lighter feedstocks within the petroleum industry continues, prices may change in such a way to make the process profitable. In particular, the transition to lighter feedstocks will likely lead to a shortage of C4, which is used as the feed to most 1,3-butadiene production processes. As the price of C4 rises in response to this shortage and the production of 1,3-butadiene becomes less economical by traditional methods, industry will move away from 1,3-butadiene production. This, in turn, can be predicted to trigger a rise in 1,3-butadiene costs due to shortage. And because lighter feedstocks will become more plentiful, propylene will be in large supply and its cost can only be predicted to fall. This falling cost of propylene and rising cost of 1,3-butadiene is very promising for our process. Even in today's market, trends already show prices moving in these directions. Figure 9.3.1 and Figure 9.3.2 below show recent market trends in pricing of 1,3-butadiene and propylene that reflect these changes.

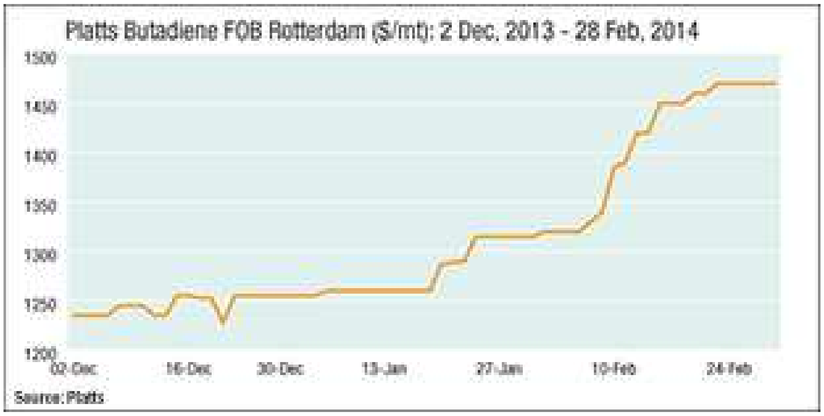


Figure 9.3.1: Graph of $/metric ton of 1,3-butadiene vs. time, showing a rising price of 1,3-butadiene

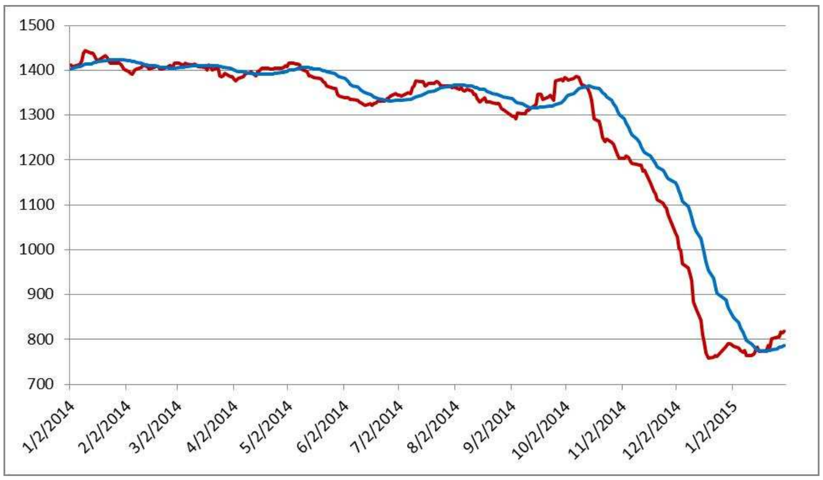


Figure 9.3.2: Graph of $/metric ton of propylene vs. time, showing a falling price of propylene

These trends can be analyzed to predict when our process will begin making profit based on the raw material (including utilities, byproduct sales, and feed costs) costs per pound of 1,3-butadiene produced. Figures 9.3.3 and 9.3.4 below reflect these prices and profitability margins by separately analyzing the response to a rising price of 1,3-butadiene or a falling price of propylene, respectively. As seen from the market predictions above, these cost trends are quite realistic and so it is expected that our process will move toward profitability in the next 20-30 years.

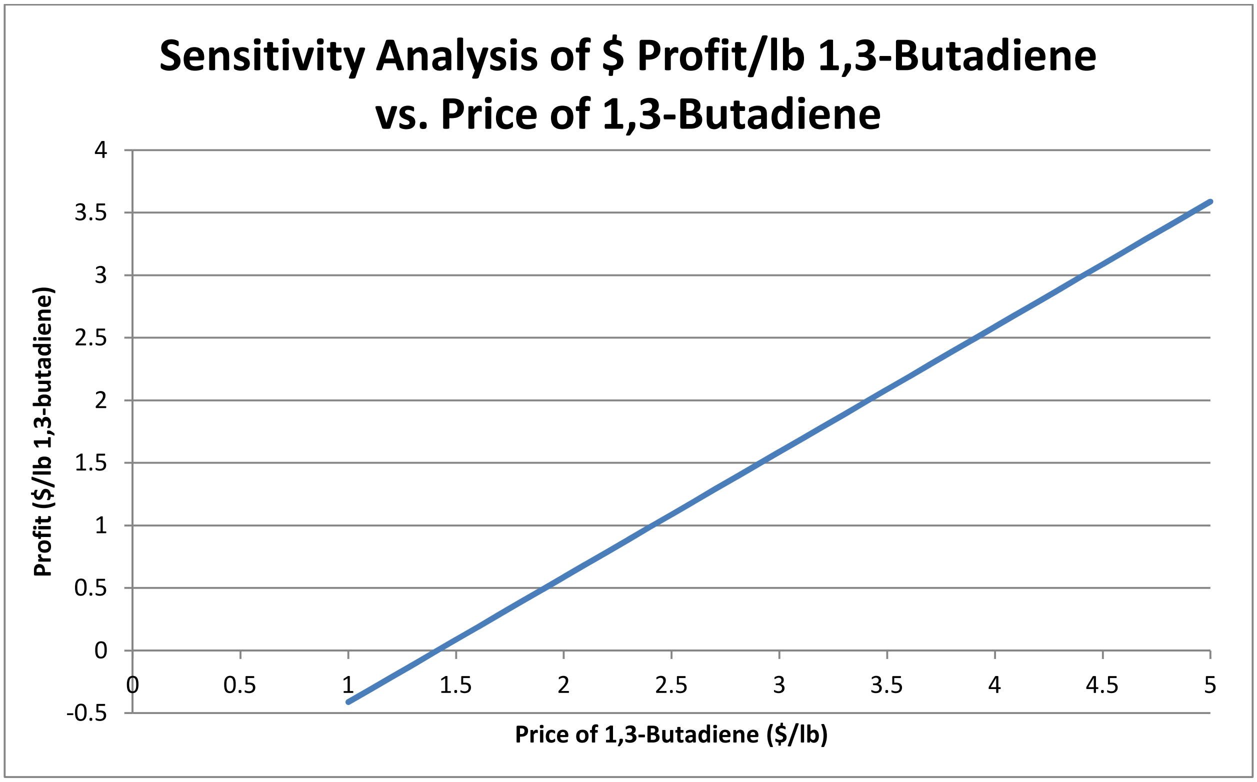


Figure 9.3.3: Sensitivity Analysis of $ Profit/lb 1,3-Butadiene vs. Price of 1,3-Butadiene

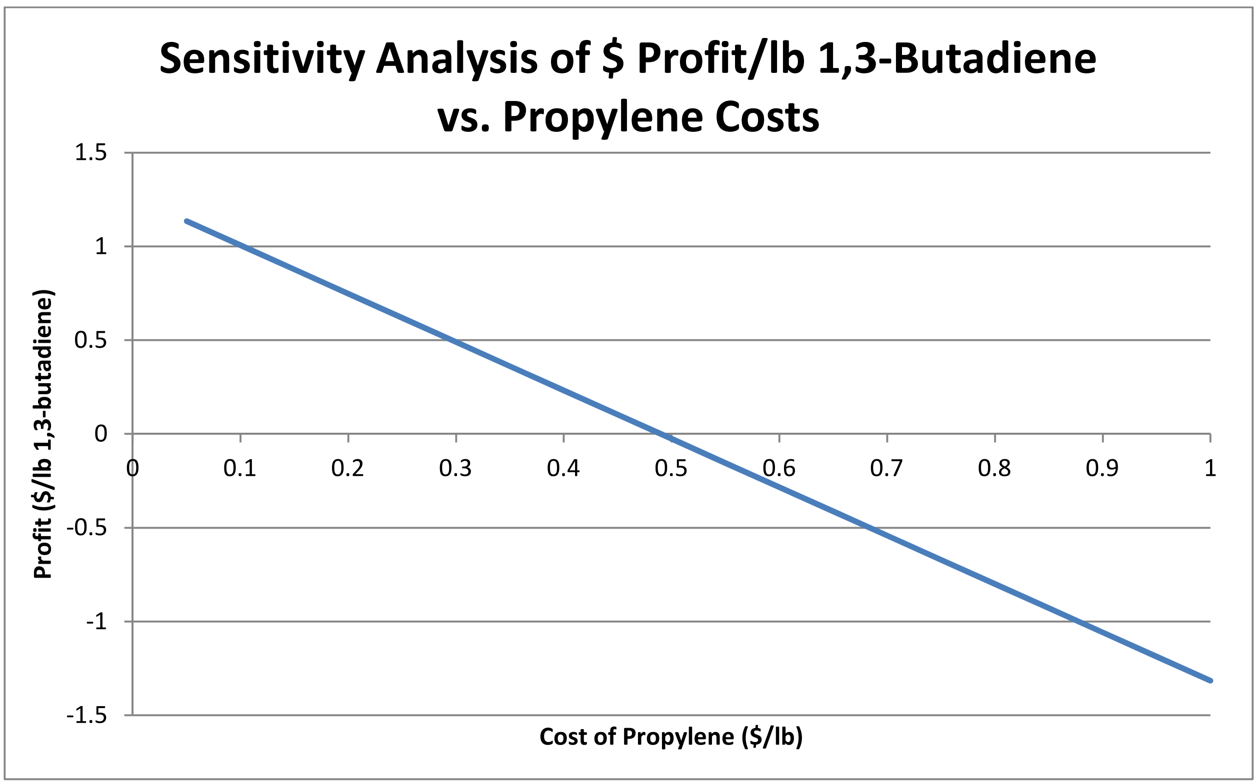


Figure 9.3.4: Sensitivity Analysis of $ Profit/lb 1,3-Butadiene vs. Propylene Costs

Analyzing the graphs above determines that we will begin making a marginal profit per pound of 1,3-butadiene produced at \$1.4/lb of 1,3-butadiene or \$0.45/lb of propylene cost. These numbers are not currently realistic, but based on market fluctuations and the predicted trends due to petroleum feedstock changes, these numbers are not an impossibility for the future. Because our current IRR was so far from profitability at current market values, this was the best method for performing a economic sensitivity analysis.

10.0 OTHER CONSIDERATIONS

Startup Considerations

The plant must be given sufficient time to reach steady state before 1,3-butadiene can be produced at full capacity. All flow rate and composition values given in this report were for steady state, however before these values can be attained several steps must be taken first.

1. Before flow can enter the first distillation train, enough mass must be accumulated so that the stream does not dry up on the stages of each column. Therefore, a storage tank must be used to accumulate effluent from the metathesis reactors before it can be introduced to the distillation train.
2. There are two recycle streams in the process, both of which must be allowed to come to steady state flow before the process flows can become constant. Each recycle stream must be handled separately:
    a. *Metathesis*: The recycle in the metathesis is comprised primarily of unreacted propylene. The storage tank prior to the distillation train should be filled to the steady state flow of 104,175 lb/hr, which will help the process accumulate enough mass flow to quickly fill the recycle stream.
    b. *Extractive Distillation*: The recycle in the extractive distillation section is almost entirely composed of the extractive solvent NMP. A pure stream of 137,246 lb/hr NMP must be fed into splitter SP-402 until the NMP has a chance to reach its steady-state flow, at which point the NMP feed may be gradually reduced to the steady state value of 1828 lb/hr.
3. Startup heaters must be used to heat and cool streams before mass flow has reached the point where stream heat exchangers can be used (H-101 and H-302).
4. All pumping and compression powers must be adjusted for smaller flows initially before mass flows have reached steady state.

5. All reactor vessels must be heated to their isothermal operating conditions before reactions can proceed at such a rate to require cooling.
6. The main feed to the system is propylene, which is continuously fed to the system at a rate of 33,664.5 lb/hr, which equates to 5,655,636 lb/week of propylene. Because propylene is a gas at room temperature, it must be stored in a pressurized vessel at the feed conditions of 73.4 °F and 364.7 psia. To reduce the requirements of the storage facility, only a week's worth of feed will be stored at a time, which may be delivered to the facility by barge or railcar.

Plant startup costs will be considerable, estimated at about 10% of the total depreciable capable of the facility. The time for the plant to reach steady-state must also be considered, and may take as much as a week.

Environmental Concerns and Waste Disposal

The plant produces a large quantity of wastewater, most of which is either spent cooling water that must have excess heat removed, or water produced during the extractive distillation that has small traces (<0.2% by wt) of hydrocarbons and must be treated before disposal. After this water is treated and cooled in a water treatment facility, it may be discharged to a local water source. Water treatment facilities that can perform this will be common on the gulf coast, where the plant is to be built. Aside from the wastewater, most waste streams in the plant can either be sold as a gasoline product (mixture of low-weight hydrocarbons) or sold as a byproduct (such as the ethylene and NMP streams). There are four additional waste streams that do not fit into any of the mentioned categories due to their composition, and so these streams will be incinerated for heat generation and vented to the atmosphere. Due to environmental concerns, some CO_2 scrubbing may have to occur before the flue gas from this procedure can be vented.

The removal of carbon deposits in the oxidative dehydrogenation vessel and the decoking process in the metathesis reactors will also have considerable waste removal requirements. The removal of carbon deposits can be done with steam, creating carbon dioxide and carbon monoxide that will likely require scrubbing before release to the atmosphere. The decoking process can either be done mechanically using water or with nitrogen, in either case which extensive treatment will be required before disposal can occur.

Health and Safety Concerns

Most of the process is comprised of hydrocarbon streams. Hydrocarbons are highly combustible and so flammability concerns are a major issue. Preventative and detective measures must be taken against leaks and electrical equipment should be kept far from major process components to avoid risks of sparking.

Most streams and units operate at high temperatures in the plant, and so human operators must take caution to avoid burns when handling or working nearby equipment. Many units also operate at high pressure, and so operators should exercise extreme caution when working with these units, as the power of high-pressure impact if any parts become detached or leaks occur could be life-threatening. Most equipment in the process is also large and heavy, and so general caution should be taken, particularly of any moving parts or protrusions, when nearby equipment.

Most hydrocarbons, while not deadly, are still not recommended for skin contact, and so protective gear should be worn whenever working with or near these products. NMP is a large health concern, as the chemical is toxic to humans and easily enters the body through skin absorption or by breathing in NMP vapors. NMP causes skin, eye, nose, and throat irritation. It affects the nervous system and can cause temporary headache, nausea, dizziness, clumsiness, and drowsiness. Frequent overexposure to NMP can cause more serious, possibly permanent effects on the nervous system and should be avoided. NMP is known to be toxic to the reproductive system, and could be toxic to other organ systems as well, but the effects in humans are still not fully understood. Exposure to NMP should be avoided at all costs, and the facility must take protective measures to avoid exposure, leaks, and other forms of contact with the chemical.

<u>Process Control</u>

This process requires numerous control valves and feedback monitors to control the various pressures and temperatures of each stream and vessel. Because most of these control systems are electronic, computer systems and software will be necessary to monitor the system. The mechanical and electrical systems involved in the control of this system have not been factored into its design or costs. The mechanical implementation of these control valves and feedback monitors will result in slight pressure drops from the tabulated values in this report. Pump and compressor horsepower will have to be adjusted to compensate for these pressure drops, and will increase utility requirements, which in turn will increase utility costs.

11.0 CONCLUSIONS

The production of 1,3-butadiene from propylene via oxidative dehydrogenation and olefin metathesis is a novel process design for 1,3-butadiene production. After careful analysis, it has been concluded that the process would not be a profitable one. The plant has a negative ROI of 202.95%, clearly indicating that the process is not profitable. The total capital investment is unsurprising for a plant of this magnitude $17,944,000, and the total fixed costs are fairly low at $1,760,402. The main loss of profitability is in the total variable costs, which amount to $200,958,000. This is a very significant amount and ultimately makes our process unprofitable.

Theoretically, this process is more desirable than traditional production methods for 1,3-butadiene due to the use of propylene, a light feedstock, as the primary feed. As the natural gas industry shifts toward lighter feedstocks, the typical feedstocks for 1,3-butadiene are being depleted. Based on this, processes for making 1,3-butadiene from lighter feedstocks will become necessary as heavy feedstocks, such as C_4, disappear. However, because these predictions are not currently reflected in the prices and trends of industry, propylene is a more costly feed than butene, making the metathesis section of this process immediately unprofitable. It is in this that our process's profitability inherently fails: it is based on predicted market trends that have yet to come into fruition, and so using current prices for raw materials and products already cost $1.83/lb of 1,3-butadiene produced. With the sale price of 1,3-butadiene at $1.00/lb and minimal revenue from byproducts, this process is inherently unprofitable.

At today's prices, the production of 1,3-butadiene from propylene is unprofitable. However, if market trends to lighter feedstocks continue, this process could become profitable. As the acquisition of butene becomes more difficult and its cost rises, the production of 1,3-butadiene through traditional methods will become more costly. If the production of 1,3-butadiene becomes less profitable, industries will not invest in its production. However, 1,3-butadiene is an essential ingredient in rubber and a number of other products commonly used in the U.S. today, making demand for it high. Therefore, as industries move away from production of 1,3-butadiene, its cost will increase. Furthermore, with the trend to lighter feedstocks, propylene supply will likely increase, resulting in a drop in price. Considering all of these market trends, it is certainly possible that the production of 1,3-butadiene from propylene become profitable in the future. Therefore, we concluded that this process should not be abandoned entirely, but rather considered for the future while factoring in market trends.

Keeping in mind that this process may become profitable at some future date, we have constructed a number of recommendations on the system to aid in profitability and understanding of this process. First, in order to better understand and model this process, extensive research must be done on the metathesis reaction, particularly in finding a catalyst to increase yield and selectivity. Our catalyst recommendations suggest targeting a propylene conversion at or above 36.24% and an isomerization conversion of 2-butene at or below 10%, preferably at or below 3% if possible. A good starting point for catalyst research is with the WO_3/SiO_2 catalyst doped with sodium used by Phillips Petroleum Co. in 1996. Once the catalyst is constructed, lab work should be able to provide more extensive data on the kinetics of the metathesis process, which can then be further optimized.

Second, methods for reducing utility requirements should be implemented. Utility costs for this process ended up being very high. A large portion of this cost comes from heating and cooling requirements, some of which required refrigerant or high-pressure steam, and high energy requirements, most of which came from compressors. Propane refrigerant was required in two condensers, making up the greatest single utility cost in the system. Alternate method to traditional distillation should be explored for these separations. For some compressors, horsepower was slightly reduced by using multi-stage compressor; however energy requirements still ended up being our second greatest utility. Methods such as lowering the overall process pressure and reducing gas flow rate streams should be explored to reduce energy usage.

As our final suggestion, proper modeling software for the extractive distillation sequence should be explored, as evidence suggests that the binary parameters used by Aspen Plus V8.6 do not properly model extractive distillation. Extractive distillation is intended as a low-energy, low-cost, high-purity, high-recovery separation method for 1,3-butadiene, and modeling it in Aspen ended up being both costly and wasteful. This is likely for two reasons: first, extractive distillation is usually modeled with scrubbers, absorbers, strippers, quench towers, and traditional distillation towers. However, we were restricted to Aspen's Radfrac columns to model all of these components, which considering the large boiling point differences in our stream components, led to huge temperature differences across columns and rigorous condenser and reboiler requirements. Second, Aspen lacked the binary parameters between the solvent, NMP, and the components it was separating, namely cis- and trans-2-butene, and therefore the parameters had to be estimated. Even with these estimations, however, the Aspen model behaved fairly differently than was prescribed by the literature, and in many ways the inclusion of the solvent actually made the separation and purification of 1,3-butadiene more difficult in Aspen. Based on these results, we would recommend finding different methods for modeling the extractive distillation section of this process, which we expect to behave differently in reality than as it is modeled in this report.

In today's market, the production of 1,3-butadiene from propylene is not a profitable process. However, as the petroleum industry moves toward lighter feedstocks and the market reacts to these changes, it is very possible that costs of propylene and 1,3-butadiene will be reflected in such a way that the process may become profitable. So while we cannot recommend construction of this plant now, the process has the potential to be feasible in the future.

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APPENDIX A: PROBLEM STATEMENT

10. Butadiene from Propylene
(recommended by Gary Sawyer, Consultant – formerly ARCO, Lyondell-Basell)

Background. The natural gas boom in the United States has led to a shift in lighter feedstocks for olefin steam crackers. Olefin crackers make ethylene, propylene, and heavier olefins from either heavy (naphtha or oil field condensates) or light (ethane/propane from natural gas condensates) feedstocks. Butadiene is an important ingredient in synthetic rubber, among other products. It is typically extracted from olefin cracker crude C4 streams, but these streams have been reduced with the trend to lighter feedstocks.

Several processes for making butadiene are available,[1] one of which involves the dehydrogenation of butane, the Houdry process. However, this still requires a C4 molecule.

Propylene is made from steam cracking as mentioned above, but recently capacity in the US has been added involving the dehydrogenation of propane (e.g., PetroLogistics). Propylene can be converted to 2-butene and ethylene through the specialized metathesis[2] reaction. The basic chemistry in a vapor phase, equilibrium-limited reaction, is:

$$\text{C-C=C} + \text{C-C=C} \Leftrightarrow \text{C-C=C-C} + \text{C=C}$$

More generally, the reaction exchanges the double bonds as:

$$R_1\text{-C=C-}R_2 + R_3\text{-C=C-}R_4 \Rightarrow \begin{array}{c} R_1\text{-C-C-}R_2 \\ |\quad | \\ R_3\text{-C-C-}R_4 \end{array} \Rightarrow R_1\text{-C=C-}R_3 + R_2\text{-C=C-}R_4$$

If the metathesis catalyst is very selective, then the only products are 2-butene and ethylene. If there is olefin isomerization such that 2-butene becomes 1-butene, then 1-butene can undergo metathesis to make ethylene, propylene, pentenes, and hexenes.

After the reaction products are separated, ethylene is sold as a byproduct, unreacted propylene is recycled, and the 2-butene can be further processed to make butadiene.

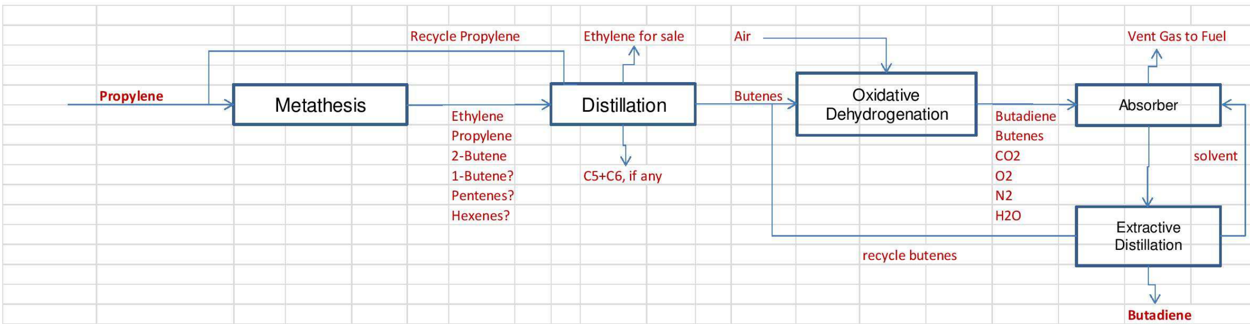
One such step to convert 2-butene to butadiene is with oxidative dehydrogenation[3]. Here, air or oxygen is added with butane(s) to a vapor-phase catalytic reactor. The basic chemistry is:

$$C_4H_8 \text{ (2-butene)} + 1/2\ O_2 \rightarrow C_4H_6 \text{ (1,3-butadiene)} + H_2O$$

---

[1] "Butadiene Product Stewardship Guidance Manual", LyondellBasell, 2010
[2] See, for example, US 8,704,029 B2 to UOP, Examples 2 and 4, figures 7 and 8.
[3] See US 20070167661 patent application to BASF, Example 2. There are many other patents and literature references on oxidative dehydrogenation to make butadiene.

The products from this reaction are cooled, condensed, and possibly absorbed in a solvent before spent air is vented. The solvent is suitable for extractive distillation to purify butadiene from unreacted 2-butene. N-methylpyrrolidone and dimethylformamide are two examples of extractive distillation solvents used in industry for butadiene purification. Figure 1 shows a block schematic of the overall process and lists some key modeling parameters for your consideration.



	Lower Bound	Typical Value	Upper Bound
Reaction Conditions			
Temperature, C		150	
Pressure, atm		2	
WHSV, (kg feed / kg catalyst/hr)		20	
Propylene conversion per pass		15%	equi-librium
Total carbon selectivity to:			
Ethylene		4%	32%
Butenes		52%	63%
Pentenes + Hexenes		44%	5%

	Lower Bound	Typical Value	Upper Bound
Reaction Conditions			
Temperature, C		400	
Pressure, atm		3	
WHSV, (kg feed / kg catalyst/hr)		1.5	
Butene conversion per pass		95%	
Butene selectivity to			
Butadiene		95%	
Combustion Products		5%	

Figure 1

Deliverables and Scope of Work. Your firm, *U Penn Process Evaluation, Inc.*, has been contracted by a major butadiene producer to develop a process model and economics that will guide their research on metathesis and oxidative dehydrogenation catalysts. The model will also be used to guide your client's Business managers on the appropriate economic climate for propylene and butadiene that would incent investment in this technology.

Review literature and set ranges on model inputs. Determine a suitable range of parameters for the tables in Figure 1 based on your review of patents and other literature you discover on the subjects. For the metathesis reaction, which is an equilibrium reaction, determine the maximum propylene conversion using Gibbs free-energy thermodynamic considerations.

Create a simplified model. Develop material balances in Excel that are updated with changing assumptions in Figure 1. Calculate profit margins (more precisely, variable margins) for different assumptions in selectivity and pricing, and summarize your results. At this stage, we are only considering the *raw material costs.* Energy, fixed costs, and investment will come later.

Develop a flowsheet. Develop a more detailed flowsheet based on your work in step 2. Decide what extractive distillation solvent you will use and why. Solvent considerations include its impact on relative volatility differences between butadiene and butane, stability at operating temperatures, susceptibility to degradation from water contamination, toxicity, and safety. In this flowsheet, you will:

a. Prepare a process flow diagram showing major equipment such as vessels, heat exchangers, and pumps.
b. Select operating pressures for key unit operations.
c. Show heating and cooling duties, and offer opportunities for heat integration.
d. Calculate compressor horsepower if gas streams are being compressed.

You may use either ASPEN PLUS or Excel to calculate heat and material balances, but the model should be able to handle reasonable changes to the Target assumptions. Again, perform an economic analysis which now includes energy and raw materials. This is essentially gives the *variable cost* of production.

Determine capital cost and final economics. Size equipment, estimate installed capital, and complete a cash-flow analysis for your selected flowsheet.

Your results will consider:

- What economic environment makes the base-case process assumptions an attractive process?
- What process parameters are needed to have an attractive process given the Economic Data below?

Additional Comments and Guidelines

- Plant Scale. Size for 100 million lb/yr of butadiene. This is roughly a 3% increase in US capacity.
- Reactor Design and Modeling. At this stage, the reactions do not need to be modeled kinetically; instead, use a stoichiometric model with conversions and yields. Be mindful of the flammable limits of butenes in air, and that these limits widen with increased pressure. Although the reactor design is eventually very important, we are looking for the big picture here. You can consider isothermal reactors such as packed

tube-in-shell designs, or adiabatic reactors with packed or fluidized beds having cooling between their stages. In the latter case, assume an allowable adiabatic temperature rise of 50°C.

- Battery Limit Conditions
  - Propylene is available as a liquid at 350 psig and ambient temperature. It is 99.5% pure with the balance as propane.
  - If you choose to use oxygen instead of air, oxygen is available at 100 psig and ambient temperature. It contains 0.5 wt% argon.
  - Butadiene must be at least 99.5% pure.

Economic Data. Your analysis will include sensitivity to pricing assumptions. Typical recent prices are:

Propylene: 65 cent/lb
Ethylene: 60 cent/lb
Butadiene: $1.00 / lb

Natural Gas: $3.50/MMBtu (InfoMine)

Electricity: 7 cent/kW-hr

Additional References

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APPENDIX B: SAMPLE CALCULATIONS

Volume of Metathesis Reactor

Volume = flow rate /density of feed/space velocity

V=104620 lb/hr/20 hr^{-1}/0.153 lb/ft^3 = **34,045 ft^3**

Mass of Catalyst

Mass = flow rate/space velocity

Mass = 104620(lb/hr)/20(kg feed/kg catalyst/hr) = **5213 lbs**

Oxydehyrogenation Tube Number Calculation

Contact time = 5s

Tube Selected = 14 BWG ¾ inch Tube

Volume of one tube = Area* Height = 0.268in^2*158 in/5s=8.4 in^3/s

Volumetric Flow Rate in the Reactor = 28.69 ft^3/s =0.004 ft^3/s

Number of Tubes = 28.7/0.004 = **7,175 tubes**

Pressure Drop and Distillation Column Sizing

$$\frac{\Delta p}{L} = \frac{150\mu(1-\varepsilon)^2 u_o}{\varepsilon^3 d_p^2} + \frac{1.75(1-\varepsilon)\rho u_0^2}{\varepsilon^3 d_p}$$

ASSUMPTIONS	METATHESIS	OXYDEHY
Viscosity (Pa.s)	7.4E-05	8.0E-06
Void fraction, ε	0.4	0.4
Length of bed (m)	16	22
Dp (m)	6.35E-03	6.35E-03
Volumetric flow rate(m^3/s)	5.2	0.26
Area (m^2)	30.1	28.3
density (kg/m^3)	2.46	9.52
superficial velocity (m/s)	0.17	9.17E-3
Pressure Drop (Pa)	3800	56
Diameter (ft)	**20.3**	**19.7**
Column Height (ft)	**52.5**	**72.2**
Space Above and Below (ft)	8	8
Manholes (ft)	6	6
Total height (ft)	**66**	**86**

These diameter and heights were fed into the costing worksheet to obtain prices.

<u>Sample Storage Tank Calculation</u>

T-202

The flow rate was 66 ft^3/hr, assuming a hold up time of 1 day to when it reaches 70% capacity.

Volume = Hold up time*flow rate/ capacity

Volume = 66*24/0.7 = 2262 ft^3 = **16,920 gal**

<u>Heat Exchanger Calculation</u>

H-302

$T_{h,in}$= 752 F

$T_{h,out}$= 449 F

$T_{c,in}$= 143 F

$T_{c,out}$= 485 F

$Q=U*A*\Delta T_{lm}$

ΔT_{lm} = 285

Q=5,873,000 btu/hr

U=200 btu/F-ft^2-hr

Ff=0.93

Area = 110 ft^3

Aspen Calculated Result = 100 ft^3

<u>Rigorous Heat Exchanger Calculation</u>

Using the calculations in Sieder et al:

$Cp= C_b*F_l*F_m*F_p$

Cb=14250

Fm=2

Fl=1

Fp=1.0496

Cost of Purchase: $28, 500 – This is greater than the value Aspen calculated. Aspen IPE values were used for consistency purposes.

<u>Cooling Water Utility Requirement</u>

Usage = Heat Duty [BTU/hr]/Heating (Cooling) Value [BTU/lb]

(This same formula was applied to calculate steam and propane requirements)

For condenser D-202,

Usage = 18750000/29.93 = **626000 lb/hr** of Cooling Water

APPENDIX C: ECONOMIC ANALYSIS TABLES

Table C.1: Summary of Economic Analysis Inputs

General Information

Process Title:	**Propylene to 1,3 Butadiene**
Product:	**1,3 Butadiene**
Plant Site Location:	**Gulf Coast, US**
Site Factor:	**1.00**
Operating Hours per Year:	**7919**
Operating Days Per Year:	**330**
Operating Factor:	**0.9040**

Product Information

This Process will Yield

	13,050	lb of 1,3 Butadiene per hour
	313,206	lb of 1,3 Butadiene per day
	103,345,387	lb of 1,3 Butadiene per year
Price	**$1.00**	**/lb**

Chronology

Year	Action	Distribution of Permanent Investment	Production Capacity	Depreciation 20 year MACRS	Product Price
2015	Design		0.0%		
2016	Construction	100%	0.0%		
2017	Construction	0%	0.0%		
2018	Construction	0%	0.0%		
2019	Production	0%	45.0%	3.75%	$1.00
2020	Production		67.5%	7.22%	$1.02
2021	Production		90.0%	6.68%	$1.04
2022	Production		90.0%	6.18%	$1.06
2023	Production		90.0%	5.71%	$1.08
2024	Production		90.0%	5.29%	$1.10
2025	Production		90.0%	4.89%	$1.13
2026	Production		90.0%	4.52%	$1.15
2027	Production		90.0%	4.46%	$1.17
2028	Production		90.0%	4.46%	$1.20
2029	Production		90.0%	4.46%	$1.22

Table C2: Variable Cost Summary

Variable Cost Summary				
Variable Costs at 100% Capacity:				
General Expenses				
	Selling / Transfer Expenses:			$ 3,100,362
	Direct Research:			$ 7,234,177
	Allocated Research:			$ 516,727
	Administrative Expense:			$ 2,066,908
	Management Incentive Compensation:			$ 1,291,817
Total General Expenses				$ 14,209,991
Raw Materials		$1.887000	per lb of 1,3 Butadiene	$195,012,746
Byproducts		$0.692250	per lb of 1,3 Butadiene	($71,540,844)
Utilities		$0.219152	per lb of 1,3 Butadiene	$22,648,307
Total Variable Costs				**$ 160,330,199**

Table C3: Fixed Cost Summary

Fixed Cost Summary		
Operations		
	Direct Wages and Benefits	$ 416,000
	Direct Salaries and Benefits	$ 62,400
	Operating Supplies and Services	$ 24,960
	Technical Assistance to Manufacturing	$ 300,000
	Control Laboratory	$ 325,000
	Total Operations	**$ 1,128,360**
Maintenance		
	Wages and Benefits	$ 172,628
	Salaries and Benefits	$ 43,157
	Materials and Services	$ 172,628
	Maintenance Overhead	$ 8,631
	Total Maintenance	**$ 397,045**
Operating Overhead		
	General Plant Overhead:	$ 49,287
	Mechanical Department Services:	$ 16,660
	Employee Relations Department:	$ 40,957
	Business Services:	$ 51,370

	Total Operating Overhead	**$**	**158,274**
Property Taxes and Insurance			
	Property Taxes and Insurance:	$	76,724
Other Annual Expenses			
	Rental Fees (Office and Laboratory Space):	$	-
	Licensing Fees:	$	-
	Miscellaneous:	$	-
	Total Other Annual Expenses	**$**	**-**
Total Fixed Costs		**$**	**1,760,402**

Table C4: Investment Summary

Investment Summary				
Installed Equipment Costs:				
	Total Direct Materials and Labor Costs	$	100,500	
	Miscellaneous Installation Costs	$	2,500,300	
	Material and Labor G&A Overhead and Contractor Fees	$	-	
	Contractor Engineering Costs	$	-	
	Indirect Costs	$	-	
	Total:			**$ 2,600,800**
Direct Permanent Investment				
	Cost of Site Preparations:	$	390,120	
	Cost of Service Facilities:	$	260,080	
	Allocated Costs for utility plants and facilities:	$	-	
	Direct Permanent Investment			**$ 3,251,000**
Total Depreciable Capital				
	Cost of Contingencies & Contractor Fees	$	585,180	
	Total Depreciable Capital			**$ 3,836,180**

Total Permanent Investment			
	Cost of Land:	$ 76,724	
	Cost of Royalties:	$ -	
	Cost of Plant Start-Up:	$ 383,618	
	Total Permanent Investment - Unadjusted		$ 4,296,522
	Site Factor		1.00
	Total Permanent Investment		**$ 4,296,522**

Table C5: Summary of Working Capital

Working Capital				
		2018	**2019**	**2020**
	Accounts Receivable	$ 3,822,364	$ 1,911,182	$ 1,911,182
	Cash Reserves	$ 902,788	$ 451,394	$ 451,394
	Accounts Payable	$ (8,050,477)	$ (4,025,239)	$ (4,025,239)
	1,3 Butadiene Inventory	$ 509,648	$ 254,824	$ 254,824
	Raw Materials	$ 480,853	$ 240,427	$ 240,427
	Total	**$ (2,334,824)**	**$ (1,167,412)**	**$ (1,167,412)**
	Present Value at 15%	*$ (1,535,185)*	*$ (667,472)*	*$ (580,410)*
Total Capital Investment			**$ 1,513,455**	

APPENDIX D: ASPEN STREAM REPORTS

SECTION 100: METATHESIS

```
S-101
 -----

 STREAM ID                S-101
 FROM :                   ----
 TO   :                   M-101

 SUBSTREAM: MIXED
 PHASE:                   LIQUID
 COMPONENTS: LBMOL/HR
   PROPYLEN              800.0000
   ETHYLENE                0.0
   TRAN-BUT                0.0
   CIS-BUT                 0.0
   1-BUTENE                0.0
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6                  0.0
   TRANS-C6                0.0
   CIS-C5                  0.0
   TRANS-C5                0.0
   NMP                     0.0
 COMPONENTS: LB/HR
   PROPYLEN             3.3665+04
   ETHYLENE                0.0
   TRAN-BUT                0.0
   CIS-BUT                 0.0
   1-BUTENE                0.0
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6                  0.0
   TRANS-C6                0.0
   CIS-C5                  0.0
   TRANS-C5                0.0
   NMP                     0.0
 COMPONENTS: MASS FRAC
   PROPYLEN                1.0000
   ETHYLENE                0.0
   TRAN-BUT                0.0
   CIS-BUT                 0.0
   1-BUTENE                0.0
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6                  0.0
   TRANS-C6                0.0
   CIS-C5                  0.0
   TRANS-C5                0.0
   NMP                     0.0
 TOTAL FLOW:
   LBMOL/HR              800.0000
   LB/HR                3.3665+04
   CUFT/HR              1075.5438
 STATE VARIABLES:
   TEMP   F               73.4000
   PRES   PSIA           364.6959
   VFRAC                   0.0
   LFRAC                   1.0000
   SFRAC                   0.0
 ENTHALPY:
   BTU/LBMOL            1878.3439
   BTU/LB                 44.6368
   BTU/HR               1.5027+06
 ENTROPY:
   BTU/LBMOL-R           -51.3008
   BTU/LB-R               -1.2191
 DENSITY:
   LBMOL/CUFT              0.7438
   LB/CUFT                31.3000
 AVG MW                   42.0806
```

SECTION 100: METATHESIS

S-205

STREAM ID	S-205		
FROM :	D-202		
TO :	M-101		
SUBSTREAM: MIXED			
PHASE:	LIQUID		
COMPONENTS: LBMOL/HR			
PROPYLEN	1250.1543		
ETHYLENE	0.5073		
TRAN-BUT	180.5193		
CIS-BUT	94.5168		
1-BUTENE	43.5289		
1:3BUTAD	0.0		
CO2	0.0		
O2	0.0		
N2	0.0		
H20	0.0		
CIS-C6	5.8254-04		
TRANS-C6	2.3407-03		
CIS-C5	0.3452		
TRANS-C5	1.0443		
NMP	0.0		
COMPONENTS: LB/HR			
PROPYLEN	5.2607+04		
ETHYLENE	14.2317		
TRAN-BUT	1.0128+04		
CIS-BUT	5303.1048		
1-BUTENE	2442.2980		
1:3BUTAD	0.0		
CO2	0.0		
O2	0.0		
N2	0.0		
H20	0.0		
CIS-C6	4.9027-02		
TRANS-C6	0.1970		
CIS-C5	24.2075		
TRANS-C5	73.2415		
NMP	0.0		
COMPONENTS: MASS FRAC			
PROPYLEN	0.7452		
ETHYLENE	2.0160-04		
TRAN-BUT	0.1435		
CIS-BUT	7.5122-02		
1-BUTENE	3.4597-02		
1:3BUTAD	0.0		
CO2	0.0		
O2	0.0		
N2	0.0		
H20	0.0		

CIS-C6	6.9451-07
TRANS-C6	2.7906-06
CIS-C5	3.4292-04
TRANS-C5	1.0375-03
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	1570.6190
LB/HR	7.0593+04
CUFT/HR	2567.3371
STATE VARIABLES:	
TEMP F	139.3177
PRES PSIA	300.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	758.4411
BTU/LB	16.8745
BTU/HR	1.1912+06
ENTROPY:	
BTU/LBMOL-R	-51.9244
BTU/LB-R	-1.1553
DENSITY:	
LBMOL/CUFT	0.6118
LB/CUFT	27.4966
AVG MW	44.9460

SECTION 100: METATHESIS

S-201

STREAM ID	S-201
FROM :	H-101
TO :	D-201
MAX CONV. ERROR:	-9.8264-06
SUBSTREAM: MIXED	
PHASE:	MIXED
COMPONENTS: LBMOL/HR	
PROPYLEN	1266.9723
ETHYLENE	413.3152
TRAN-BUT	360.5766
CIS-BUT	221.5652
1-BUTENE	65.7786
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	0.2718
TRANS-C6	1.1450
CIS-C5	10.5330
TRANS-C5	30.4608
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	5.3315+04
ETHYLENE	1.1595+04
TRAN-BUT	2.0231+04
CIS-BUT	1.2431+04
1-BUTENE	3690.6750
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	22.8791
TRANS-C6	96.3686
CIS-C5	738.7261
TRANS-C5	2136.3508
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	0.5114
ETHYLENE	0.1112
TRAN-BUT	0.1940
CIS-BUT	0.1192
1-BUTENE	3.5400-02
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	2.1945-04
TRANS-C6	9.2433-04
CIS-C5	7.0856-03
TRANS-C5	2.0491-02
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	2370.6187
LB/HR	1.0426+05
CUFT/HR	2.2874+04
STATE VARIABLES:	
TEMP F	179.0030
PRES PSIA	400.0000
VFRAC	0.7687
LFRAC	0.2313
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	6603.5527
BTU/LB	150.1522
BTU/HR	1.5655+07
ENTROPY:	
BTU/LBMOL-R	-42.1447
BTU/LB-R	-0.9583
DENSITY:	
LBMOL/CUFT	0.1036
LB/CUFT	4.5580
AVG MW	43.9791

SECTION 200: DISTILLATION

```
S-201
 -----

 STREAM ID                S-201
 FROM :                   H-101
 TO   :                   D-201


 MAX CONV. ERROR:      -9.8264-06
 SUBSTREAM: MIXED
 PHASE:                   MIXED
 COMPONENTS: LBMOL/HR
   PROPYLEN             1266.9723
   ETHYLENE              413.3152
   TRAN-BUT              360.5766
   CIS-BUT               221.5652
   1-BUTENE               65.7786
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6                  0.2718
   TRANS-C6                1.1450
   CIS-C5                 10.5330
   TRANS-C5               30.4608
   NMP                     0.0
 COMPONENTS: LB/HR
   PROPYLEN             5.3315+04
   ETHYLENE             1.1595+04
   TRAN-BUT             2.0231+04
   CIS-BUT              1.2431+04
   1-BUTENE             3690.6750
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6                 22.8791
   TRANS-C6               96.3686
   CIS-C5                738.7261
   TRANS-C5             2136.3508
   NMP                     0.0
 COMPONENTS: MASS FRAC
   PROPYLEN                0.5114
   ETHYLENE                0.1112
   TRAN-BUT                0.1940
   CIS-BUT                 0.1192
   1-BUTENE             3.5400-02
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6               2.1945-04
   TRANS-C6             9.2433-04
   CIS-C5               7.0856-03
   TRANS-C5             2.0491-02
   NMP                     0.0
 TOTAL FLOW:
   LBMOL/HR             2370.6187
   LB/HR                1.0426+05
   CUFT/HR              2.2874+04
 STATE VARIABLES:
   TEMP   F              179.0030
   PRES   PSIA           400.0000
   VFRAC                   0.7687
   LFRAC                   0.2313
   SFRAC                   0.0
 ENTHALPY:
   BTU/LBMOL            6603.5527
   BTU/LB                150.1522
   BTU/HR               1.5655+07
 ENTROPY:
   BTU/LBMOL-R           -42.1447
   BTU/LB-R               -0.9583
 DENSITY:
   LBMOL/CUFT              0.1036
   LB/CUFT                 4.5580
 AVG MW                   43.9791
```

SECTION 200: DISTILLATION

S-202

STREAM ID	S-202
FROM :	D-201
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	4.1866
ETHYLENE	412.8073
TRAN-BUT	3.0789-05
CIS-BUT	1.0930-05
1-BUTENE	3.0407-05
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	2.0818-15
TRANS-C6	7.3750-15
CIS-C5	1.9575-10
TRANS-C5	6.2207-10
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	176.1729
ETHYLENE	1.1581+04
TRAN-BUT	1.7275-03
CIS-BUT	6.1324-04
1-BUTENE	1.7061-03
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	1.7521-13
TRANS-C6	6.2069-13
CIS-C5	1.3729-08
TRANS-C5	4.3629-08
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	1.4985-02
ETHYLENE	0.9850
TRAN-BUT	1.4694-07
CIS-BUT	5.2160-08
1-BUTENE	1.4511-07
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	1.4903-17
TRANS-C6	5.2793-17
CIS-C5	1.1677-12
TRANS-C5	3.7109-12
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	416.9939
LB/HR	1.1757+04
CUFT/HR	506.1817
STATE VARIABLES:	
TEMP F	2.3160
PRES PSIA	400.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	1.7400+04
BTU/LB	617.1486
BTU/HR	7.2558+06
ENTROPY:	
BTU/LBMOL-R	-29.6299
BTU/LB-R	-1.0509
DENSITY:	
LBMOL/CUFT	0.8238
LB/CUFT	23.2268
AVG MW	28.1946

SECTION 200: DISTILLATION

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S-205
 -----

 STREAM ID                S-205
 FROM :                   D-202
 TO   :                   M-101

 SUBSTREAM: MIXED
 PHASE:                   LIQUID
 COMPONENTS: LBMOL/HR
   PROPYLEN             1250.1543
   ETHYLENE                0.5073
   TRAN-BUT              180.5193
   CIS-BUT                94.5168
   1-BUTENE               43.5289
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6               5.8254-04
   TRANS-C6             2.3407-03
   CIS-C5                  0.3452
   TRANS-C5                1.0443
   NMP                     0.0
 COMPONENTS: LB/HR
   PROPYLEN             5.2607+04
   ETHYLENE               14.2317
   TRAN-BUT             1.0128+04
   CIS-BUT              5303.1048
   1-BUTENE             2442.2980
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6               4.9027-02
   TRANS-C6                0.1970
   CIS-C5                 24.2075
   TRANS-C5               73.2415
   NMP                     0.0
 COMPONENTS: MASS FRAC
   PROPYLEN                0.7452
   ETHYLENE             2.0160-04
   TRAN-BUT                0.1435
   CIS-BUT              7.5122-02
   1-BUTENE             3.4597-02
   1:3BUTAD                0.0
   CO2                     0.0
   O2                      0.0
   N2                      0.0
   H20                     0.0
   CIS-C6               6.9451-07
   TRANS-C6             2.7906-06
   CIS-C5               3.4292-04
   TRANS-C5             1.0375-03
   NMP                     0.0
 TOTAL FLOW:
   LBMOL/HR             1570.6190
   LB/HR                7.0593+04
   CUFT/HR              2567.3371
 STATE VARIABLES:
   TEMP   F              139.3177
   PRES   PSIA           300.0000
   VFRAC                   0.0
   LFRAC                   1.0000
   SFRAC                   0.0
 ENTHALPY:
   BTU/LBMOL             758.4411
   BTU/LB                 16.8745
   BTU/HR               1.1912+06
 ENTROPY:
   BTU/LBMOL-R           -51.9244
   BTU/LB-R               -1.1553
 DENSITY:
   LBMOL/CUFT              0.6118
   LB/CUFT                27.4966
 AVG MW                   44.9460
```

SECTION 200: DISTILLATION

S-208

STREAM ID	S-208
FROM :	D-203
TO :	H-302
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	12.6307
ETHYLENE	8.9670-05
TRAN-BUT	178.5335
CIS-BUT	125.3447
1-BUTENE	22.1802
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	2.8466-03
TRANS-C6	1.1281-02
CIS-C5	3.0341
TRANS-C5	9.2290
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	531.5067
ETHYLENE	2.5156-03
TRAN-BUT	1.0017+04
CIS-BUT	7032.7799
1-BUTENE	1244.4771
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	0.2396
TRANS-C6	0.9494
CIS-C5	212.7948
TRANS-C5	647.2734
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	2.6998-02
ETHYLENE	1.2778-07
TRAN-BUT	0.5088
CIS-BUT	0.3572
1-BUTENE	6.3213-02
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	1.2169-05
TRANS-C6	4.8227-05
CIS-C5	1.0809-02
TRANS-C5	3.2878-02
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	350.9665
LB/HR	1.9687+04
CUFT/HR	577.8002
STATE VARIABLES:	
TEMP F	142.7479
PRES PSIA	100.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.1203+04
BTU/LB	-199.7150
BTU/HR	-3.9318+06
ENTROPY:	
BTU/LBMOL-R	-72.2122
BTU/LB-R	-1.2873
DENSITY:	
LBMOL/CUFT	0.6074
LB/CUFT	34.0725
AVG MW	56.0940

SECTION 200: DISTILLATION

S-209

STREAM ID	S-209
FROM :	D-203
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	1.5237-04
ETHYLENE	4.2101-12
TRAN-BUT	1.5243
CIS-BUT	1.7040
1-BUTENE	6.9753-02
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	0.2684
TRANS-C6	1.1314
CIS-C5	7.1538
TRANS-C5	20.1876
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	6.4118-03
ETHYLENE	1.1811-10
TRAN-BUT	85.5264
CIS-BUT	95.6047
1-BUTENE	3.9137
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	22.5908
TRANS-C6	95.2231
CIS-C5	501.7275
TRANS-C5	1415.8469
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	2.8876-06
ETHYLENE	5.3191-14
TRAN-BUT	3.8518-02
CIS-BUT	4.3057-02
1-BUTENE	1.7626-03
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	1.0174-02
TRANS-C6	4.2885-02
CIS-C5	0.2260
TRANS-C5	0.6376
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	32.0395
LB/HR	2220.4394
CUFT/HR	66.1137
STATE VARIABLES:	
TEMP F	217.2624
PRES PSIA	102.8800
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.8372+04
BTU/LB	-265.1024
BTU/HR	-5.8864+05
ENTROPY:	
BTU/LBMOL-R	-89.0477
BTU/LB-R	-1.2849
DENSITY:	
LBMOL/CUFT	0.4846
LB/CUFT	33.5852
AVG MW	69.3032

SECTION 300: OXIDATIVE DEHYDROGENATION

S-208

STREAM ID	S-208
FROM :	D-203
TO :	H-302
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	12.6307
ETHYLENE	8.9670-05
TRAN-BUT	178.5335
CIS-BUT	125.3447
1-BUTENE	22.1802
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	2.8466-03
TRANS-C6	1.1281-02
CIS-C5	3.0341
TRANS-C5	9.2290
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	531.5067
ETHYLENE	2.5156-03
TRAN-BUT	1.0017+04
CIS-BUT	7032.7799
1-BUTENE	1244.4771
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	0.2396
TRANS-C6	0.9494
CIS-C5	212.7948
TRANS-C5	647.2734
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	2.6998-02
ETHYLENE	1.2778-07
TRAN-BUT	0.5088
CIS-BUT	0.3572
1-BUTENE	6.3213-02
1:3BUTAD	0.0
CO2	0.0
O2	0.0
N2	0.0
H20	0.0
CIS-C6	1.2169-05
TRANS-C6	4.8227-05
CIS-C5	1.0809-02
TRANS-C5	3.2878-02
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	350.9665
LB/HR	1.9687+04
CUFT/HR	577.8002
STATE VARIABLES:	
TEMP F	142.7479
PRES PSIA	100.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.1203+04
BTU/LB	-199.7150
BTU/HR	-3.9318+06
ENTROPY:	
BTU/LBMOL-R	-72.2122
BTU/LB-R	-1.2873
DENSITY:	
LBMOL/CUFT	0.6074
LB/CUFT	34.0725
AVG MW	56.0940

SECTION 300: OXIDATIVE DEHYDROGENATION

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S-304
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 STREAM ID                 S-304
 FROM :                    ----
 TO   :                    C-301

 SUBSTREAM: MIXED
 PHASE:                    VAPOR
 COMPONENTS: LBMOL/HR
   PROPYLEN                  0.0
   ETHYLENE                  0.0
   TRAN-BUT                  0.0
   CIS-BUT                   0.0
   1-BUTENE                  0.0
   1:3BUTAD                  0.0
   CO2                       0.0
   O2                      236.4600
   N2                      889.5400
   H20                       0.0
   CIS-C6                    0.0
   TRANS-C6                  0.0
   CIS-C5                    0.0
   TRANS-C5                  0.0
   NMP                       0.0
 COMPONENTS: LB/HR
   PROPYLEN                  0.0
   ETHYLENE                  0.0
   TRAN-BUT                  0.0
   CIS-BUT                   0.0
   1-BUTENE                  0.0
   1:3BUTAD                  0.0
   CO2                       0.0
   O2                     7566.4362
   N2                     2.4919+04
   H20                       0.0
   CIS-C6                    0.0
   TRANS-C6                  0.0
   CIS-C5                    0.0
   TRANS-C5                  0.0
   NMP                       0.0
 COMPONENTS: MASS FRAC
   PROPYLEN                  0.0
   ETHYLENE                  0.0
   TRAN-BUT                  0.0
   CIS-BUT                   0.0
   1-BUTENE                  0.0
   1:3BUTAD                  0.0
   CO2                       0.0
   O2                        0.2329
   N2                        0.7671
   H20                       0.0
   CIS-C6                    0.0
   TRANS-C6                  0.0
   CIS-C5                    0.0
   TRANS-C5                  0.0
   NMP                       0.0
 TOTAL FLOW:
   LBMOL/HR               1126.0000
   LB/HR                  3.2486+04
   CUFT/HR                4.3405+05
 STATE VARIABLES:
   TEMP   F                 68.0000
   PRES   PSIA              14.6959
   VFRAC                     1.0000
   LFRAC                     0.0
   SFRAC                     0.0
 ENTHALPY:
   BTU/LBMOL               -63.7329
   BTU/LB                   -2.2091
   BTU/HR                -7.1763+04
 ENTROPY:
   BTU/LBMOL-R               0.9000
   BTU/LB-R               3.1196-02
 DENSITY:
   LBMOL/CUFT             2.5942-03
   LB/CUFT                7.4842-02
 AVG MW                     28.8504
```

SECTION 300: OXIDATIVE DEHYDROGENATION

S-308

STREAM ID	S-308
FROM :	H-302
TO :	F-401
SUBSTREAM: MIXED	
PHASE:	VAPOR
COMPONENTS: LBMOL/HR	
PROPYLEN	12.6307
ETHYLENE	8.9670-05
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	22.1802
1:3BUTAD	288.6843
CO2	60.7756
O2	0.9544
N2	889.5400
H20	349.4599
CIS-C6	2.8466-03
TRANS-C6	1.1281-02
CIS-C5	3.0341
TRANS-C5	9.2290
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	531.5067
ETHYLENE	2.5156-03
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1244.4771
1:3BUTAD	1.5615+04
CO2	2674.7238
O2	30.5394
N2	2.4919+04
H20	6295.6186
CIS-C6	0.2396
TRANS-C6	0.9494
CIS-C5	212.7948
TRANS-C5	647.2734
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	1.0187-02
ETHYLENE	4.8216-08
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	2.3853-02
1:3BUTAD	0.2993
CO2	5.1267-02
O2	5.8535-04
N2	0.4776
H20	0.1207
CIS-C6	4.5919-06
TRANS-C6	1.8198-05
CIS-C5	4.0787-03
TRANS-C5	1.2406-02
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	1636.5025
LB/HR	5.2173+04
CUFT/HR	5.4567+04
STATE VARIABLES:	
TEMP F	485.2516
PRES PSIA	300.0000
VFRAC	1.0000
LFRAC	0.0
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.5849+04
BTU/LB	-497.1292
BTU/HR	-2.5937+07
ENTROPY:	
BTU/LBMOL-R	-7.0621
BTU/LB-R	-0.2215
DENSITY:	
LBMOL/CUFT	2.9991-02
LB/CUFT	0.9561
AVG MW	31.8806

SECTION 400: Extractive Distillation

S-308

STREAM ID	S-308
FROM :	H-302
TO :	F-401
SUBSTREAM: MIXED	
PHASE:	VAPOR
COMPONENTS: LBMOL/HR	
PROPYLEN	12.6307
ETHYLENE	8.9670-05
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	22.1802
1:3BUTAD	288.6843
CO2	60.7756
O2	0.9544
N2	889.5400
H20	349.4599
CIS-C6	2.8466-03
TRANS-C6	1.1281-02
CIS-C5	3.0341
TRANS-C5	9.2290
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	531.5067
ETHYLENE	2.5156-03
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1244.4771
1:3BUTAD	1.5615+04
CO2	2674.7238
O2	30.5394
N2	2.4919+04
H20	6295.6186
CIS-C6	0.2396
TRANS-C6	0.9494
CIS-C5	212.7948
TRANS-C5	647.2734
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	1.0187-02
ETHYLENE	4.8216-08
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	2.3853-02
1:3BUTAD	0.2993
CO2	5.1267-02
O2	5.8535-04
N2	0.4776
H20	0.1207
CIS-C6	4.5919-06
TRANS-C6	1.8198-05
CIS-C5	4.0787-03
TRANS-C5	1.2406-02
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	1636.5025
LB/HR	5.2173+04
CUFT/HR	5.4567+04
STATE VARIABLES:	
TEMP F	485.2516
PRES PSIA	300.0000
VFRAC	1.0000
LFRAC	0.0
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.5849+04
BTU/LB	-497.1292
BTU/HR	-2.5937+07
ENTROPY:	
BTU/LBMOL-R	-7.0621
BTU/LB-R	-0.2215
DENSITY:	
LBMOL/CUFT	2.9991-02
LB/CUFT	0.9561
AVG MW	31.8806

SECTION 400: Extractive Distillation

S-418

```
 STREAM ID                S-418
 FROM :                   ----
 TO   :                   M-403

 SUBSTREAM: MIXED
 PHASE:                   LIQUID
 COMPONENTS: LBMOL/HR
   PROPYLEN                 0.0
   ETHYLENE                 0.0
   TRAN-BUT                 0.0
   CIS-BUT                  0.0
   1-BUTENE                 0.0
   1:3BUTAD                 0.0
   CO2                      0.0
   O2                       0.0
   N2                       0.0
   H2O                      0.0
   CIS-C6                   0.0
   TRANS-C6                 0.0
   CIS-C5                   0.0
   TRANS-C5                 0.0
   NMP                     18.4376
 COMPONENTS: LB/HR
   PROPYLEN                 0.0
   ETHYLENE                 0.0
   TRAN-BUT                 0.0
   CIS-BUT                  0.0
   1-BUTENE                 0.0
   1:3BUTAD                 0.0
   CO2                      0.0
   O2                       0.0
   N2                       0.0
   H2O                      0.0
   CIS-C6                   0.0
   TRANS-C6                 0.0
   CIS-C5                   0.0
   TRANS-C5                 0.0
   NMP                   1827.7663
 COMPONENTS: MASS FRAC
   PROPYLEN                 0.0
   ETHYLENE                 0.0
   TRAN-BUT                 0.0
   CIS-BUT                  0.0
   1-BUTENE                 0.0
   1:3BUTAD                 0.0
   CO2                      0.0
   O2                       0.0
   N2                       0.0
   H2O                      0.0
   CIS-C6                   0.0
   TRANS-C6                 0.0
   CIS-C5                   0.0
   TRANS-C5                 0.0
   NMP                      1.0000
 TOTAL FLOW:
   LBMOL/HR                18.4376
   LB/HR                 1827.7663
   CUFT/HR                 29.7000
 STATE VARIABLES:
   TEMP   F               100.0000
   PRES   PSIA             14.7000
   VFRAC                    0.0
   LFRAC                    1.0000
   SFRAC                    0.0
 ENTHALPY:
   BTU/LBMOL            -1.1383+05
   BTU/LB               -1148.2948
   BTU/HR               -2.0988+06
 ENTROPY:
   BTU/LBMOL-R           -139.1468
   BTU/LB-R                -1.4036
 DENSITY:
   LBMOL/CUFT               0.6208
   LB/CUFT                 61.5409
 AVG MW                    99.1326
```

SECTION 400: Extractive Distillation

S-405

STREAM ID	S-405
FROM :	D-401
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	1.3055-04
ETHYLENE	2.7373-11
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	3.1802-03
1:3BUTAD	1.8304-07
CO2	7.9945-06
O2	2.9836-09
N2	2.2586-06
H20	348.9117
CIS-C6	2.7814-03
TRANS-C6	1.1042-02
CIS-C5	6.6979-02
TRANS-C5	0.1737
NMP	0.0
COMPONENTS: LB/HR	
PROPYLEN	5.4938-03
ETHYLENE	7.6792-10
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	0.1784
1:3BUTAD	9.9008-06
CO2	3.5184-04
O2	9.5473-08
N2	6.3271-05
H20	6285.7417
CIS-C6	0.2341
TRANS-C6	0.9293
CIS-C5	4.6975
TRANS-C5	12.1844
NMP	0.0
COMPONENTS: MASS FRAC	
PROPYLEN	8.7149-07
ETHYLENE	1.2182-13
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	2.8305-05
1:3BUTAD	1.5706-09
CO2	5.5812-08
O2	1.5145-11
N2	1.0037-08
H20	0.9971
CIS-C6	3.7134-05
TRANS-C6	1.4742-04
CIS-C5	7.4517-04
TRANS-C5	1.9328-03
NMP	0.0
TOTAL FLOW:	
LBMOL/HR	349.1695
LB/HR	6303.9714
CUFT/HR	119.7580
STATE VARIABLES:	
TEMP F	330.6337
PRES PSIA	103.8800
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.1779+05
BTU/LB	-6524.4746
BTU/HR	-4.1130+07
ENTROPY:	
BTU/LBMOL-R	-31.5834
BTU/LB-R	-1.7494
DENSITY:	
LBMOL/CUFT	2.9156
LB/CUFT	52.6393
AVG MW	18.0542

SECTION 400: Extractive Distillation

S-407

STREAM ID	S-407
FROM :	D-402
TO :	----
SUBSTREAM: MIXED	
PHASE:	VAPOR
COMPONENTS: LBMOL/HR	
PROPYLEN	8.8518
ETHYLENE	8.3917-05
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	4.6796-03
1:3BUTAD	6.0725
CO2	57.6766
O2	0.9435
N2	880.2842
H20	1.2352-06
CIS-C6	2.7246-11
TRANS-C6	9.2506-11
CIS-C5	9.5277-06
TRANS-C5	3.0077-05
NMP	1.2652-07
COMPONENTS: LB/HR	
PROPYLEN	372.4883
ETHYLENE	2.3542-03
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	0.2626
1:3BUTAD	328.4707
CO2	2538.3350
O2	30.1898
N2	2.4660+04
H20	2.2253-05
CIS-C6	2.2931-09
TRANS-C6	7.7854-09
CIS-C5	6.6822-04
TRANS-C5	2.1095-03
NMP	1.2542-05
COMPONENTS: MASS FRAC	
PROPYLEN	1.3337-02
ETHYLENE	8.4290-08
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	9.4008-06
1:3BUTAD	1.1761-02
CO2	9.0883-02
O2	1.0809-03
N2	0.8829
H20	7.9676-10
CIS-C6	8.2101-14
TRANS-C6	2.7875-13
CIS-C5	2.3925-08
TRANS-C5	7.5528-08
NMP	4.4905-10
TOTAL FLOW:	
LBMOL/HR	953.8333
LB/HR	2.7930+04
CUFT/HR	8969.5246
STATE VARIABLES:	
TEMP F	-21.5326
PRES PSIA	500.0000
VFRAC	1.0000
LFRAC	0.0
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-1.0558+04
BTU/LB	-360.5797
BTU/HR	-1.0071+07
ENTROPY:	
BTU/LBMOL-R	-8.2940
BTU/LB-R	-0.2833
DENSITY:	
LBMOL/CUFT	0.1063
LB/CUFT	3.1138
AVG MW	29.2814

SECTION 400: Extractive Distillation

S-409

STREAM ID		S-409
FROM :		D-403
TO :		----
SUBSTREAM: MIXED		
PHASE:		VAPOR
COMPONENTS: LBMOL/HR		
	PROPYLEN	2.4952
	ETHYLENE	5.5464-06
	TRAN-BUT	0.0
	CIS-BUT	0.0
	1-BUTENE	3.2028-02
	1:3BUTAD	16.8864
	CO2	3.0052
	O2	1.0861-02
	N2	9.2074
	H20	4.7441-03
	CIS-C6	3.1666-09
	TRANS-C6	1.1546-08
	CIS-C5	4.7095-04
	TRANS-C5	1.4605-03
	NMP	3.6510-03
COMPONENTS: LB/HR		
	PROPYLEN	104.9990
	ETHYLENE	1.5560-04
	TRAN-BUT	0.0
	CIS-BUT	0.0
	1-BUTENE	1.7970
	1:3BUTAD	913.4135
	CO2	132.2567
	O2	0.3475
	N2	257.9300
	H20	8.5466-02
	CIS-C6	2.6651-07
	TRANS-C6	9.7170-07
	CIS-C5	3.3030-02
	TRANS-C5	0.1024
	NMP	0.3619
COMPONENTS: MASS FRAC		
	PROPYLEN	7.4397-02
	ETHYLENE	1.1025-07
	TRAN-BUT	0.0
	CIS-BUT	0.0
	1-BUTENE	1.2733-03
	1:3BUTAD	0.6472
	CO2	9.3711-02
	O2	2.4625-04
	N2	0.1828
	H20	6.0557-05
	CIS-C6	1.8883-10
	TRANS-C6	6.8850-10
	CIS-C5	2.3403-05
	TRANS-C5	7.2578-05
	NMP	2.5645-04
TOTAL FLOW:		
	LBMOL/HR	31.6473
	LB/HR	1411.3268
	CUFT/HR	466.5461
STATE VARIABLES:		
	TEMP F	227.1941
	PRES PSIA	500.0000
	VFRAC	1.0000
	LFRAC	0.0
	SFRAC	0.0
ENTHALPY:		
	BTU/LBMOL	1.2015+04
	BTU/LB	269.4152
	BTU/HR	3.8023+05
ENTROPY:		
	BTU/LBMOL-R	-20.8867
	BTU/LB-R	-0.4684
DENSITY:		
	LBMOL/CUFT	6.7833-02
	LB/CUFT	3.0251
AVG MW		44.5954

SECTION 400: Extractive Distillation

S-410

STREAM ID	S-410
FROM :	D-403
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	0.3746
ETHYLENE	2.0517-07
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1.3538-02
1:3BUTAD	7.0919
CO2	9.3874-02
O2	6.6037-05
N2	4.9804-02
H20	7.7949-04
CIS-C6	8.9787-09
TRANS-C6	3.3047-08
CIS-C5	6.0763-04
TRANS-C5	1.8620-03
NMP	0.2848
COMPONENTS: LB/HR	
PROPYLEN	15.7647
ETHYLENE	5.7558-06
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	0.7596
1:3BUTAD	383.6114
CO2	4.1314
O2	2.1131-03
N2	1.3952
H20	1.4043-02
CIS-C6	7.5566-07
TRANS-C6	2.7812-06
CIS-C5	4.2616-02
TRANS-C5	0.1306
NMP	28.2323
COMPONENTS: MASS FRAC	
PROPYLEN	3.6317-02
ETHYLENE	1.3260-08
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1.7498-03
1:3BUTAD	0.8837
CO2	9.5174-03
O2	4.8680-06
N2	3.2141-03
H20	3.2350-05
CIS-C6	1.7408-09
TRANS-C6	6.4071-09
CIS-C5	9.8174-05
TRANS-C5	3.0084-04
NMP	6.5039-02
TOTAL FLOW:	
LBMOL/HR	7.9118
LB/HR	434.0838
CUFT/HR	13.7605
STATE VARIABLES:	
TEMP F	227.1941
PRES PSIA	500.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	3.4173+04
BTU/LB	622.8464
BTU/HR	2.7037+05
ENTROPY:	
BTU/LBMOL-R	-43.5739
BTU/LB-R	-0.7942
DENSITY:	
LBMOL/CUFT	0.5750
LB/CUFT	31.5457
AVG MW	54.8651

SECTION 400: Extractive Distillation

S-415

STREAM ID	S-415
FROM :	D-405
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	5.4093-06
ETHYLENE	0.0
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	21.1116
1:3BUTAD	17.5850
CO2	0.0
O2	0.0
N2	0.0
H20	0.5207
CIS-C6	6.5064-05
TRANS-C6	2.3882-04
CIS-C5	2.9644
TRANS-C5	9.0470
NMP	4.2123
COMPONENTS: LB/HR	
PROPYLEN	2.2763-04
ETHYLENE	0.0
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1184.5186
1:3BUTAD	951.1999
CO2	0.0
O2	0.0
N2	0.0
H20	9.3804
CIS-C6	5.4759-03
TRANS-C6	2.0099-02
CIS-C5	207.9058
TRANS-C5	634.5048
NMP	417.5791
COMPONENTS: MASS FRAC	
PROPYLEN	6.6849-08
ETHYLENE	0.0
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	0.3479
1:3BUTAD	0.2793
CO2	0.0
O2	0.0
N2	0.0
H20	2.7548-03
CIS-C6	1.6081-06
TRANS-C6	5.9027-06
CIS-C5	6.1057-02
TRANS-C5	0.1863
NMP	0.1226
TOTAL FLOW:	
LBMOL/HR	55.4413
LB/HR	3405.1146
CUFT/HR	85.7354
STATE VARIABLES:	
TEMP F	104.7582
PRES PSIA	50.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-5836.7859
BTU/LB	-95.0332
BTU/HR	-3.2360+05
ENTROPY:	
BTU/LBMOL-R	-73.9891
BTU/LB-R	-1.2047
DENSITY:	
LBMOL/CUFT	0.6467
LB/CUFT	39.7165
AVG MW	61.4184

SECTION 400: Extractive Distillation

PRODUCT

STREAM ID	PRODUCT
FROM :	D-404
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	0.9090
ETHYLENE	1.0513-09
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1.0117
1:3BUTAD	241.0456
CO2	9.5291-05
O2	2.1480-10
N2	1.2307-07
H20	1.8309-02
CIS-C6	1.0536-08
TRANS-C6	3.7921-08
CIS-C5	8.8969-04
TRANS-C5	2.7143-03
NMP	0.1459
COMPONENTS: LB/HR	
PROPYLEN	38.2493
ETHYLENE	2.9494-08
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	56.7630
1:3BUTAD	1.3039+04
CO2	4.1937-03
O2	6.8733-09
N2	3.4477-06
H20	0.3298
CIS-C6	8.8671-07
TRANS-C6	3.1915-06
CIS-C5	6.2398-02
TRANS-C5	0.1904
NMP	14.4645
COMPONENTS: MASS FRAC	
PROPYLEN	2.9090-03
ETHYLENE	2.2431-12
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	4.3170-03
1:3BUTAD	0.9953
CO2	3.1895-07
O2	5.2274-13
N2	2.6221-10
H20	2.5086-05
CIS-C6	6.7438-11
TRANS-C6	2.4273-10
CIS-C5	4.7456-06
TRANS-C5	1.4478-05
NMP	1.1001-03
TOTAL FLOW:	
LBMOL/HR	243.1341
LB/HR	1.3149+04
CUFT/HR	403.5963
STATE VARIABLES:	
TEMP F	190.6876
PRES PSIA	200.0000
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	4.1899+04
BTU/LB	774.7652
BTU/HR	1.0187+07
ENTROPY:	
BTU/LBMOL-R	-44.4103
BTU/LB-R	-0.8212
DENSITY:	
LBMOL/CUFT	0.6024
LB/CUFT	32.5786
AVG MW	54.0797

SECTION 400: Extractive Distillation

PURGE

STREAM ID	PURGE
FROM :	SP-401
TO :	----
SUBSTREAM: MIXED	
PHASE:	LIQUID
COMPONENTS: LBMOL/HR	
PROPYLEN	6.2231-10
ETHYLENE	0.0
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	3.5097-03
1:3BUTAD	3.4150-03
CO2	0.0
O2	0.0
N2	0.0
H20	1.8528-03
CIS-C6	2.3708-08
TRANS-C6	8.6510-08
CIS-C5	7.4276-04
TRANS-C5	2.2317-03
NMP	13.7919
COMPONENTS: LB/HR	
PROPYLEN	2.6187-08
ETHYLENE	0.0
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	0.1969
1:3BUTAD	0.1847
CO2	0.0
O2	0.0
N2	0.0
H20	3.3378-02
CIS-C6	1.9953-06
TRANS-C6	7.2808-06
CIS-C5	5.2093-02
TRANS-C5	0.1565
NMP	1367.2278
COMPONENTS: MASS FRAC	
PROPYLEN	1.9145-11
ETHYLENE	0.0
TRAN-BUT	0.0
CIS-BUT	0.0
1-BUTENE	1.4396-04
1:3BUTAD	1.3505-04
CO2	0.0
O2	0.0
N2	0.0
H20	2.4402-05
CIS-C6	1.4587-09
TRANS-C6	5.3228-09
CIS-C5	3.8084-05
TRANS-C5	1.1442-04
NMP	0.9995
TOTAL FLOW:	
LBMOL/HR	13.8037
LB/HR	1367.8514
CUFT/HR	28.8761
STATE VARIABLES:	
TEMP F	503.7000
PRES PSIA	52.3300
VFRAC	0.0
LFRAC	1.0000
SFRAC	0.0
ENTHALPY:	
BTU/LBMOL	-9.3659+04
BTU/LB	-945.1608
BTU/HR	-1.2928+06
ENTROPY:	
BTU/LBMOL-R	-112.5796
BTU/LB-R	-1.1361
DENSITY:	
LBMOL/CUFT	0.4780
LB/CUFT	47.3697
AVG MW	99.0934

APPENDIX E: Material Safety Data Sheets

Propylene

Safety Data Sheet P-4648

according to U.S. Code of Federal Regulations 29 CFR 1910.1200, Hazard Communication.

Date of issue: 01/01/1983 Revision date: 04/08/2015 Supersedes: 01/13/2015

SECTION: 1. Product and company identification

1.1. Product identifier

Product form	:	Substance
Name	:	Propylene
CAS No	:	115-07-1
Formula	:	C3H6

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture	:	Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
39 Old Ridgebury Road
Danbury, CT 06810-5113 - USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number	:	Onsite Emergency: 1-800-645-4633 CHEMTREC, 24hr/day 7days/week — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887 (collect calls accepted, Contract 17729)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Gas 1 H220
Liquefied gas H280

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS02 GHS04

Signal word (GHS-US)	:	DANGER
Hazard statements (GHS-US)	:	H220 - EXTREMELY FLAMMABLE GAS H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED OSHA-H01 - MAY DISPLACE OXYGEN AND CAUSE RAPID SUFFOCATION. CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR CGA-HG01 - MAY CAUSE FROSTBITE.
Precautionary statements (GHS-US)	:	P202 - Do not handle until all safety precautions have been read and understood P210 - Keep away from Heat, Open flames, Sparks, Hot surfaces. - No smoking P271+P403 - Use and store only outdoors or in a well-ventilated place. P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely P381 - Eliminate all ignition sources if safe to do so CGA-PG05 - Use a back flow preventive device in the piping. CGA-PG12 - Do not open valve until connected to equipment prepared for use. CGA-PG06 - Close valve after each use and when empty. CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles. CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

Other hazards not contributing to the classification : Contact with liquid may cause cold burns/frostbite.

2.4. Unknown acute toxicity (GHS US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%
Propylene (Main constituent)	(CAS No) 115-07-1	100

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.

First-aid measures after skin contact : The liquid may cause frostbite. For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

. Adverse effects not expected from this product.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately. Get immediate medical attention.

First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.

Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.

Reactivity : No reactivity hazard other than the effects described in sub-sections below.

5.3. Advice for firefighters

Firefighting instructions : Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.

Protection during firefighting : Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.

Special protective equipment for fire fighters : Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.

Specific methods : Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems.

Stop flow of product if safe to do so.

Use water spray or fog to knock down fire fumes if possible.

Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Eliminate ignition sources. Evacuate area. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous. Wear self-contained breathing apparatus when entering area unless atmosphere is proven to be safe. Ensure adequate ventilation. Stop leak if safe to do so.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Try to stop release. Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.

Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post "No Smoking or Open Flames" signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Propylene (115-07-1)		
ACGIH	ACGIH TLV-TWA (ppm)	500 ppm
USA OSHA	Not established	

8.2. Exposure controls

Appropriate engineering controls : During welding, ensure that there is adequate ventilation to keep worker exposure below applicable limits for fumes, gases, and other by-products of welding. Do not breathe fumes or gases. Short-term overexposure to fumes may cause dizziness, nausea, and dryness or irritation of the nose, throat, and eyes, or may cause other similar discomfort. Use an explosion-proof local exhaust system. Local exhaust and general ventilation must be adequate to meet exposure standards. MECHANICAL (GENERAL): **Inadequate - Use only in a closed system.** Use explosion proof equipment and lighting.

Hand protection : Wear working gloves when handling gas containers. Wear work gloves when handling containers; welding gloves for welding. Gloves must be free of oil and grease.

Eye protection : Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections. Wear safety glasses with side shields.

Respiratory protection : When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure (e.g., an organic vapor cartridge). For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).

Thermal hazard protection : Wear cold insulating gloves when transfilling or breaking transfer connections.

Environmental exposure controls : Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment.

Other information : Wear safety shoes while handling containers. Consider the use of flame resistant anti-static safety clothing. Wear leather safety gloves and safety shoes when handling cylinders.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Gas

Appearance : Colorless gas.

Molecular mass : 42 g/mol

Color : Colorless.

Odor	: Stenchant often added. Sweetish.
Odor threshold	: Odour threshold is subjective and inadequate to warn for overexposure.
pH	: Not applicable.
Relative evaporation rate (butyl acetate=1)	: No data available
Relative evaporation rate (ether=1)	: Not applicable.
Melting point	: No data available
Freezing point	: -185.25 °C (-301.45°F)
Boiling point	: -47.72 °C (-53.9°F)
Flash point	: -107.8 °C (-162°F)
Critical temperature	: 91.8 °C (197.24°F)
Auto-ignition temperature	: 455 °C (851°F)
Decomposition temperature	: No data available
Flammability (solid, gas)	: 2 - 11.1
Vapor pressure	: 10.2 bar (132.81 psig) @70°F (21.1 °C), 1 ATM
Relative vapor density at 20 °C	: No data available
Relative density	: 0.6
Density	: 0.5139 g/cm³ (at 20 °C)
Relative gas density	: 1.5
Solubility	: Water: 384 mg/l
Log Pow	: 1.77
Log Kow	: Not applicable.
Viscosity, kinematic	: Not applicable.
Viscosity, dynamic	: Not applicable.
Explosive properties	: Not applicable.
Oxidizing properties	: None.
Explosion limits	: No data available

9.2. Other information

Gas group	: Liquefied gas
Additional information	: Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Can form explosive mixture with air. May react violently with oxidants.

10.4. Conditions to avoid

Keep away from heat/sparks/open flames/hot surfaces. – No smoking.

10.5. Incompatible materials

Oxidizing agent. Acids. Halogens.

10.6. Hazardous decomposition products

Thermal decomposition or burning may produce carbon monoxide, carbon dioxide, and hydrogen. The welding and cutting process may form reaction products such as carbon monoxide and carbon dioxide. Other decomposition products of normal operation originate from the volatilization, reaction, or oxidation of the material being worked.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Propylene (\f)115-07-1	
LC50 inhalation rat (mg/l)	658 mg/l/4h
ATE US (vapors)	658.000 mg/l/4h
ATE US (dust, mist)	658.000 mg/l/4h

Skin corrosion/irritation : Not classified

pH: Not applicable.

Serious eye damage/irritation : Not classified

pH: Not applicable.

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Propylene (115-07-1)	
IARC group	3 - Not classifiable

Reproductive toxicity : Not classified

Specific target organ toxicity (single exposure) : Not classified

Specific target organ toxicity (repeated exposure) : Not classified

Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No ecological damage caused by this product.

12.2. Persistence and degradability

Propylene (115-07-1)	
Persistence and degradability	The substance is biodegradable. Unlikely to persist.

12.3. Bioaccumulative potential

Propylene (115-07-1)	
Log Pow	1.77
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

12.4. Mobility in soil

Propylene (115-07-1)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

SECTION 14: Transport information

In accordance with DOT

Transport document description	: UN1077 Propylene, 2.1
UN-No.(DOT)	: UN1077
Proper Shipping Name (DOT)	: Propylene
Transport hazard class(es) (DOT)	: 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115
Hazard labels (DOT)	: 2.1 - Flammable gas

DOT Special Provisions (49 CFR 172.102)	: 19 - For domestic transportation only, the identification number UN1075 may be used in place of the identification number specified in column (4) of the 172.101 table. The identification number used must be consistent on package markings, shipping papers and emergency response information. T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

Additional information

Emergency Response Guide (ERG) Number	: 115 (UN1075)
Other information	: No supplementary information available.
Special transport precautions	: Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers: - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG)	: 1077
Proper Shipping Name (IMDG)	: PROPYLENE
Class (IMDG)	: 2 - Gases
MFAG-No	: 115

Air transport

UN-No.(IATA)	: 1077
Proper Shipping Name (IATA)	: Propylene
Class (IATA)	: 2
Civil Aeronautics Law	: Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

Propylene (115-07-1)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory Listed on United States SARA Section 313	
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Fire hazard Sudden release of pressure hazard Delayed (chronic) health hazard
SARA Section 313 - Emission Reporting	1.0 %

All components of this product are listed on the Toxic Substances Control Act (TSCA) inventory.

	Chemical(s) subject to the reporting requirements of Section 313 or Title III of the Superfund Amendments and Reauthorization Act (SARA) of 1986 and 40 CFR Part 372.	
Propylene	CAS No 115-07-1	100%

15.2. International regulations

CANADA

Propylene (115-07-1)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

Propylene (115-07-1)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

15.2.2. National regulations

Propylene (115-07-1)
Listed on the AICS (Australian Inventory of Chemical Substances) Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China) Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory Listed on the Korean ECL (Existing Chemicals List) Listed on NZIoC (New Zealand Inventory of Chemicals) Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

15.3. US State regulations

Propylene(115-07-1)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List U.S. - Pennsylvania - RTK (Right to Know) List

California Proposition 65 - This product contains, or may contain, trace quantities of a substance(s) known to the state of California to cause cancer and/or reproductive toxicity

SECTION 16: Other information

Revision date : 4/8/2015 12:00:00 AM

Other information : When using this product in welding and cutting, read and understand the manufacturer's instructions and the precautionary label on the product. Ask your welding products supplier for a copy of Praxair's free safety booklet, P-2035, Precautions and Safe Practices for Gas Welding, Cutting, and Heating, and for other manufacturers' safety publications. For a detailed treatment, get ANSI Z49.1, Safety in Welding, Cutting, and Allied Processes, published by the American Welding Society (AWS), www.aws.org. Order AWS documents from Global Engineering Documents, global.ihs.com. Arcs and sparks can ignite combustible materials. Prevent fires. Refer to NFPA 51B, Standard for Fire Prevention During Welding, Cutting, and Other Hotwork. Do not strike an arc on the container. The defect produced by an arc burn may lead to container rupture.

Fumes and gases produced during welding and cutting processes can be dangerous to your health and may cause serious lung disease. KEEP YOUR HEAD OUT OF FUMES. DO NOT BREATHE FUMES AND GASES. Use enough ventilation, local exhaust, or both to keep fumes and gases from your breathing zone and the general area. Short-term overexposure to fumes may cause dizziness, nausea, and dryness or irritation of the nose, throat, and eyes; or may cause other similar discomfort. Contaminants in the air may add to the hazard of fumes and gases.

When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc., it is the user's obligation to determine the conditions of safe use of the product.

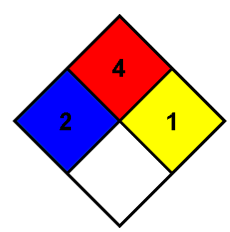
Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc., P.O. Box 44, Tonawanda, NY 14151-0044).

PRAXAIR and the Flowing Airstream design are trademarks or registered trademarks of Praxair Technology, Inc. in the United States and/or other countries.

NFPA health hazard : 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.

NFPA fire hazard : 4 - Will rapidly or completely vaporize at normal pressure and temperature, or is readily dispersed in air and will burn readily.

NFPA reactivity : 1 - Normally stable, but can become unstable at elevated temperatures and pressures or may react with water with some release of energy, but not violently.



HMIS III Rating

Health : 1 Slight Hazard - Irritation or minor reversible injury possible

Flammability : 4 Severe Hazard

Physical : 2 Moderate Hazard

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

Ethylene

Safety Data Sheet P-4598

according to U.S. Code of Federal Regulations 29 CFR 1910.1200, Hazard Communication.

Date of issue: 01/01/1979 Revision date: 03/03/2015 Supersedes: 12/01/2009

SECTION: 1. Product and company identification

1.1. Product identifier

Product form	:	Substance
Name	:	Ethylene
CAS No	:	74-85-1
Formula	:	C2H4
Other means of identification	:	Ethene, Acetene, Olefiant Gas, refrigerant gas R1150

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture	:	Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
39 Old Ridgebury Road
Danbury, CT 06810-5113 - USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number	:	Onsite Emergency: 1-800-645-4633 CHEMTREC, 24hr/day 7days/week — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887 (collect calls accepted, Contract 17729)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Gas 1 H220
Liquefied gas H280
STOT SE 3 H336

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS02 GHS04 GHS07

Signal word (GHS-US)	:	DANGER
Hazard statements (GHS-US)	:	H220 - EXTREMELY FLAMMABLE GAS H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED H336 - MAY CAUSE DROWSINESS OR DIZZINESS OSHA-H01 - MAY DISPLACE OXYGEN AND CAUSE RAPID SUFFOCATION. CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR CGA-HG01 - MAY CAUSE FROSTBITE.
Precautionary statements (GHS-US)	:	P202 - Do not handle until all safety precautions have been read and understood P210 - Keep away from Heat, Open flames, Sparks, Hot surfaces. - No smoking P261 - Avoid breathing gas P262 - Do not get in eyes, on skin, or on clothing. P271+P403 - Use and store only outdoors or in a well-ventilated place. P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely P381 - Eliminate all ignition sources if safe to do so CGA-PG05 - Use a back flow preventive device in the piping. CGA-PG12 - Do not open valve until connected to equipment prepared for use. CGA-PG06 - Close valve after each use and when empty.

CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles.
CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

Other hazards not contributing to the classification : Contact with liquid may cause cold burns/frostbite.

2.4. Unknown acute toxicity (GHS-US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%
Ethylene (Main constituent)	(CAS No) 74-85-1	100

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : Immediately remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, qualified personnel may give oxygen. Call a physician.

First-aid measures after skin contact : For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.

First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None. Obtain medical assistance.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.

Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.

Reactivity : No reactivity hazard other than the effects described in sub-sections below.

5.3. Advice for firefighters

Firefighting instructions : **DANGER: FLAMMABLE LIQUID AND VAPOR.** Evacuate all personnel from danger area. Use self-contained breathing apparatus. Immediately cool surrounding containers with water spray from maximum distance, taking care not to extinguish flames. Avoid spreading burning liquid with water. Remove ignition sources if safe to do so. If flames are accidentally extinguished, explosive reignition may occur. Reduce vapors with water spray or fog. Stop flow of liquid if safe to do so, while continuing cooling water spray. Remove all containers from area of fire if safe to do so. Allow fire to burn out. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1919 Subpart L - Fire Protection.

Special protective equipment for fire fighters	: Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.
Other information	: Containers are equipped with a pressure relief device. (Exceptions may exist where authorized by DOT.).

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: **DANGER: Flammable liquid and gas under pressure.** Forms explosive mixtures with air. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Try to stop release. Reduce vapor with fog or fine water spray. Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.

Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post "No Smoking or Open Flames" signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Ethylene (74-85-1)		
ACGIH	ACGIH TLV-TWA (ppm)	200 ppm
ACGIH	Remark (ACGIH)	Asphyxia
USA OSHA	Not established	

8.2. Exposure controls

Appropriate engineering controls : Use an explosion-proof local exhaust system. Local exhaust and general ventilation must be adequate to meet exposure standards. MECHANICAL (GENERAL): Inadequate - Use only in a closed system. Use explosion proof equipment and lighting.

Eye protection : Wear safety glasses when handling cylinders; vapor-proof goggles and a face shield during cylinder changeout or whenever contact with product is possible. Select eye protection in accordance with OSHA 29 CFR 1910.133.

Skin and body protection : Wear metatarsal shoes and work gloves for cylinder handling, and protective clothing where needed. Wear neoprene gloves during cylinder changeout or wherever contact with product is possible. Select per OSHA 29 CFR 1910.132, 1910.136, and 1910.138.

Respiratory protection : When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure (e.g., an organic vapor cartridge). For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA). Self contained breathing apparatus (SCBA) or positive pressure airline with mask are to be used in oxygen-deficient atmospheres.

Thermal hazard protection : Wear cold insulating gloves when transfilling or breaking transfer connections.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Gas

Appearance : Colorless gas.

Molecular mass : 28 g/mol

Color : Colorless.

Odor : Sweetish.

Odor threshold : No data available

pH	: Not applicable.
Relative evaporation rate (butyl acetate=1)	: No data available
Relative evaporation rate (ether=1)	: Not applicable.
Melting point	: -169 °C
Freezing point	: No data available
Boiling point	: -102.4 °C (at 700 mmHg)
Flash point	: -136.1 °C TCC
Critical temperature	: 9.6 °C
Auto-ignition temperature	: 450 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: 2.7 - 36 vol %
Vapor pressure	: Not applicable.
Critical pressure	: 5041 kPa
Relative vapor density at 20 °C	: No data available
Relative density	: 0.57
Specific gravity / density	: 0.974 g/cm³ (at 15 °C)
Relative gas density	: 0.975
Solubility	: Water: 130 mg/l
Log Pow	: 1.13
Log Kow	: Not applicable.
Viscosity, kinematic	: Not applicable.
Viscosity, dynamic	: Not applicable.
Explosive properties	: Not applicable.
Oxidizing properties	: None.
Explosive limits	: No data available

9.2. Other information

Gas group	: Liquefied gas
Additional information	: None.

SECTION 10: Stability and reactivity

10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

May occur.

10.4. Conditions to avoid

May decompose violently at high temperature and/or pressure or in the presence of a catalyst.

10.5. Incompatible materials

Oxidizing agents. Halogens. Halogenated compounds. Chlorine. Acids. Aluminum chloride.

10.6. Hazardous decomposition products

Thermal decomposition may produce : Carbon dioxide. Carbon monoxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Skin corrosion/irritation : Not classified
pH: Not applicable.

Serious eye damage/irritation : Not classified
pH: Not applicable.

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Ethylene (74-85-1)	
IARC group	3 - Not classifiable

Reproductive toxicity : Not classified

Specific target organ toxicity (single exposure) : MAY CAUSE DROWSINESS OR DIZZINESS.

Specific target organ toxicity (repeated exposure) : Not classified

Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No known ecological damage caused by this product.

12.2. Persistence and degradability

Ethylene (74-85-1)	
Persistence and degradability	The substance is biodegradable. Unlikely to persist.

12.3. Bioaccumulative potential

Ethylene (74-85-1)	
BCF fish 1	4 - 4.6
Log Pow	1.13
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

12.4. Mobility in soil

Ethylene (74-85-1)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Do not attempt to dispose of residual or unused quantities. Return container to supplier.

SECTION 14: Transport information

In accordance with DOT

Transport document description : UN1962 Ethylene, 2.1

UN-No.(DOT) : UN1962

Proper Shipping Name (DOT) : Ethylene

Department of Transportation (DOT) Hazard Classes : 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115

Hazard labels (DOT) : 2.1 - Flammable gas

Additional information

Emergency Response Guide (ERG) Number : 115 (UN1038);116P (UN1962)

Other information : No supplementary information available.

Special transport precautions : Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers: - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG) : 1962
Proper Shipping Name (IMDG) : ETHYLENE
Class (IMDG) : 2 - Gases
MFAG-No : 116P

Air transport

UN-No.(IATA) : 1962
Proper Shipping Name (IATA) : Ethylene
Class (IATA) : 2
Civil Aeronautics Law : Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

Ethylene (74-85-1)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory Listed on United States SARA Section 313	
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Sudden release of pressure hazard Fire hazard
SARA Section 313 - Emission Reporting	1.0 %

15.2. International regulations

CANADA

Ethylene (74-85-1)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

Ethylene (74-85-1)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

15.2.2. National regulations

Ethylene (74-85-1)
Listed on the AICS (Australian Inventory of Chemical Substances) Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China) Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory Listed on the Korean ECL (Existing Chemicals List) Listed on NZIoC (New Zealand Inventory of Chemicals) Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

15.3. US State regulations

Ethylene(74-85-1)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

Revision date : 3/3/2015 12:00:00 AM

Other information : When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc., it is the user's obligation to determine the conditions of safe use of the product.

Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc., P.O. Box 44, Tonawanda, NY 14151-0044).

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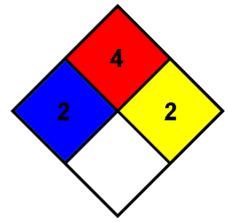
NFPA health hazard	: 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.
NFPA fire hazard	: 4 - Will rapidly or completely vaporize at normal pressure and temperature, or is readily dispersed in air and will burn readily.
NFPA reactivity	: 2 - Normally unstable and readily undergo violent decomposition but do not detonate. Also: may react violently with water or may form potentially explosive mixtures with water.



HMIS III Rating

Health	: 1 Slight Hazard - Irritation or minor reversible injury possible
Flammability	: 4 Severe Hazard
Physical	: 3 Serious Hazard

SDS US (GHS HazCom 2012) - Praxair

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

trans-2-Butene

Safety Data Sheet P-4578

according to U.S. Code of Federal Regulations 29 CFR 1910.1200, Hazard Communication.

Date of issue: 01/01/1979 Revision date: 01/27/2015 Supersedes: 12/01/2009

SECTION: 1. Product and company identification

1.1. Product identifier

Product form	:	Substance
Name	:	trans-2-Butene
CAS No	:	624-64-6
Formula	:	C4H8
Other means of identification	:	trans-2-Butene

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture : Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
39 Old Ridgebury Road
Danbury, CT 06810-5113 - USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number : Onsite Emergency: 1-800-645-4633

CHEMTREC, 24hr/day 7days/week — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887 (collect calls accepted, Contract 17729)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Gas 1 H220
Liquefied gas H280

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :


GHS02


GHS04

Signal word (GHS-US) : DANGER

Hazard statements (GHS-US) :
H220 - EXTREMELY FLAMMABLE GAS
H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED
OSHA-H01 - MAY DISPLACE OXYGEN AND CAUSE RAPID SUFFOCATION.
CGA-HG01 - MAY CAUSE FROSTBITE.
CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR

Precautionary statements (GHS-US) :
P202 - Do not handle until all safety precautions have been read and understood
P210 - Keep away from heat, Open flames, sparks, hot surfaces. - No smoking
P271+P403 - Use and store only outdoors or in a well-ventilated place.
P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely
P381 - Eliminate all ignition sources if safe to do so
CGA-PG05 - Use a back flow preventive device in the piping.
CGA-PG12 - Do not open valve until connected to equipment prepared for use.
CGA-PG06 - Close valve after each use and when empty.
CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles.
CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

No additional information available

2.4. Unknown acute toxicity (GHS-US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%
trans-2-Butene (Main constituent)	(CAS No) 624-64-6	100

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.

First-aid measures after skin contact : For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.

First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.

Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.

5.3. Advice for firefighters

Firefighting instructions : Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.

Protection during firefighting : Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.

Special protective equipment for fire fighters : Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.

Specific methods : Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems.

Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Forms explosive mixtures with air. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Isolate from cylinders of oxygen and chlorine.

This gas is heavier than air and in an enclosed space tends to accumulate near the floor, displacing air and pushing it upward. This creates an oxygen-deficient atmosphere near the floor. Ventilate space before entry. Verify sufficient oxygen concentration.

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.

Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post "No Smoking or Open Flames" signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

trans-2-Butene (624-64-6)		
ACGIH	ACGIH TLV-TWA (ppm)	250 ppm
USA OSHA	Not established	

8.2. Exposure controls

Appropriate engineering controls : Use an explosion-proof local exhaust system with sufficient flow velocity to maintain an adequate supply of air in the worker's breathing zone. Mechanical/General measures: Use in a closed system.

Eye protection : Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections. Wear safety glasses with side shields.

Skin and body protection : Wear metatarsal shoes and work gloves for cylinder handling, and protective clothing where needed. Wear neoprene gloves during cylinder changeout or wherever contact with product is possible. Select per OSHA 29 CFR 1910.132, 1910.136, and 1910.138.

Respiratory protection : When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure (e.g., an organic vapor cartridge). For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).

Thermal hazard protection : Wear cold insulating gloves when transfilling or breaking transfer connections.

Environmental exposure controls : Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Gas

Molecular mass : 56 g/mol

Color : Colorless.

Odor : Sweetish.

Odor threshold : Odor threshold is subjective and inadequate to warn for overexposure.

pH : Not applicable.

Relative evaporation rate (butyl acetate=1) : No data available

Relative evaporation rate (ether=1)	:	Not applicable.
Melting point	:	105 °C
Freezing point	:	No data available
Boiling point	:	0.88 °C
Flash point	:	-73 °C TCC
Critical temperature	:	155.4 °C
Auto-ignition temperature	:	324 °C
Decomposition temperature	:	No data available
Flammability (solid, gas)	:	1.6 - 9.7 vol %
Vapor pressure	:	200 kPa
Critical pressure	:	3985 kPa
Relative vapor density at 20 °C	:	No data available
Relative density	:	0.63
Relative gas density	:	2
Solubility	:	Water: No data available
Log Pow	:	2.32
Log Kow	:	Not applicable.
Viscosity, kinematic	:	Not applicable.
Viscosity, dynamic	:	Not applicable.
Explosive properties	:	Not applicable.
Oxidizing properties	:	None.
Explosive limits	:	No data available

9.2. Other information

Gas group	:	Liquefied gas
Additional information	:	Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous polymerization may occur if normal conditions are exceeded. This material is a flammable hydrocarbon and may explode in the presence of oxidizers.

10.4. Conditions to avoid

Keep away from heat/sparks/open flames/hot surfaces. – No smoking.

10.5. Incompatible materials

Oxidizing agent. Halogens. Acids.

10.6. Hazardous decomposition products

Thermal decomposition may produce : Carbon dioxide. Carbon monoxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity	:	Not classified
Skin corrosion/irritation	:	Not classified pH: Not applicable.

Serious eye damage/irritation : Not classified
pH: Not applicable.
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified

Reproductive toxicity : Not classified
Specific target organ toxicity (single exposure) : Not classified

Specific target organ toxicity (repeated exposure) : Not classified
No known effects from this product.

Aspiration hazard : Not classified
Not applicable.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No data available. No ecological damage caused by this product.

12.2. Persistence and degradability

trans-2-Butene (624-64-6)	
Persistence and degradability	No ecological damage caused by this product.

12.3. Bioaccumulative potential

trans-2-Butene (624-64-6)	
Log Pow	2.32
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

12.4. Mobility in soil

trans-2-Butene (624-64-6)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

SECTION 14: Transport information

In accordance with DOT
Transport document description : UN1075 Petroleum gases, liquefied, 2.1
UN-No.(DOT) : UN1075
Proper Shipping Name (DOT) : Petroleum gases, liquefied
Department of Transportation (DOT) Hazard Classes : 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115

Hazard labels (DOT) : 2.1 - Flammable gas

DOT Special Provisions (49 CFR 172.102) : T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

Additional information

Other information : No supplementary information available.

Special transport precautions : Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers: - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG) : 1012
Proper Shipping Name (IMDG) : PETROLEUM GASES, LIQUEFIED
Class (IMDG) : 2 - Gases
MFAG-No : 115

Air transport

UN-No.(IATA) : 1012
Proper Shipping Name (IATA) : Petroleum gases, liquefied
Class (IATA) : 2
Civil Aeronautics Law : Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

trans-2-Butene (624-64-6)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory	
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Sudden release of pressure hazard Fire hazard

15.2. International regulations

CANADA

trans-2-Butene (624-64-6)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

trans-2-Butene (624-64-6)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Flam. Gas 1 H220
Liquefied gas H280

Full text of H-phrases: see section 16

15.2.2. National regulations

trans-2-Butene (624-64-6)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

15.3. US State regulations

trans-2-Butene(624-64-6)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

Revision date : 1/27/2015 12:00:00 AM

Other information : When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc., it is the user's obligation to determine the conditions of safe use of the product.

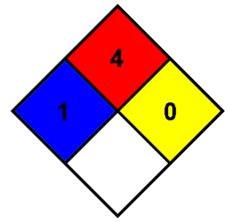
Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc., P.O. Box 44, Tonawanda, NY 14151-0044).

PRAXAIR and the Flowing Airstream design are trademarks or registered trademarks of Praxair Technology, Inc. in the United States and/or other countries.

Full text of H-phrases:

Flam. Gas 1	Flammable gases Category 1
Liquefied gas	Gases under pressure Liquefied gas
H220	EXTREMELY FLAMMABLE GAS
H280	CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED

NFPA health hazard	: 1 - Exposure could cause irritation but only minor residual injury even if no treatment is given.
NFPA fire hazard	: 4 - Will rapidly or completely vaporize at normal pressure and temperature, or is readily dispersed in air and will burn readily.
NFPA reactivity	: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

Health	: 0 Minimal Hazard - No significant risk to health
Flammability	: 4 Severe Hazard
Physical	: 1 Slight Hazard

SDS US (GHS HazCom 2012) - Praxair

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

Making our planet more productive™

cis-2-Butene

Safety Data Sheet P-4577

according to U.S. Code of Federal Regulations 29 CFR 1910.1200, Hazard Communication.

Date of issue: 01/01/1979 Revision date: 02/20/2015 Supersedes: 12/01/2009

SECTION: 1. Product and company identification

1.1. Product identifier

Product form	:	Substance
Name	:	cis-2-Butene
CAS No	:	590-18-1
Formula	:	C4H8

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture	:	Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
39 Old Ridgebury Road
Danbury, CT 06810-5113 - USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number	:	Onsite Emergency: 1-800-645-4633 CHEMTREC, 24hr/day 7days/week — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887 (collect calls accepted, Contract 17729)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Gas 1 H220
Liquefied gas H280

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS02 GHS04

Signal word (GHS-US)	:	DANGER
Hazard statements (GHS-US)	:	H220 - EXTREMELY FLAMMABLE GAS H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED OSHA-H01 - MAY DISPLACE OXYGEN AND CAUSE RAPID SUFFOCATION. CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR CGA-HG01 - MAY CAUSE FROSTBITE.
Precautionary statements (GHS-US)	:	P202 - Do not handle until all safety precautions have been read and understood P210 - Keep away from heat, Open flames, sparks, hot surfaces. - No smoking P271+P403 - Use and store only outdoors or in a well-ventilated place. P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely P381 - Eliminate all ignition sources if safe to do so CGA-PG05 - Use a back flow preventive device in the piping. CGA-PG12 - Do not open valve until connected to equipment prepared for use. CGA-PG06 - Close valve after each use and when empty. CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles. CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

Other hazards not contributing to the classification : None.

2.4. Unknown acute toxicity (GHS-US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%
cis-2-Butene (Main constituent)	(CAS No) 590-18-1	100

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : Remove victim to uncontaminated area wearing self contained breathing apparatus. Keep victim warm and rested. Call a doctor. Apply artificial respiration if breathing stopped.

First-aid measures after skin contact : For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.

First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.

Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.

Reactivity : No reactivity hazard other than the effects described in sub-sections below.

5.3. Advice for firefighters

Firefighting instructions : Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.

Protection during firefighting : Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.

Special protective equipment for fire fighters : Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.

Specific methods	: Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Forms explosive mixtures with air. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.

This gas is heavier than air and in an enclosed space tends to accumulate near the floor, displacing air and pushing it upward. This creates an oxygen-deficient atmosphere near the floor. Ventilate space before entry. Verify sufficient oxygen concentration.

Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post “No Smoking or Open Flames” signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

cis-2-Butene (590-18-1)		
ACGIH	ACGIH TLV-TWA (ppm)	250 ppm
USA OSHA	Not established	

8.2. Exposure controls

Appropriate engineering controls : Use an explosion-proof local exhaust system with sufficient flow velocity to maintain an adequate supply of air in the worker's breathing zone. Mechanical/General measures: Use in a closed system.

Eye protection : Wear safety glasses with side shields. Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections.

Skin and body protection : Wear metatarsal shoes and work gloves for cylinder handling, and protective clothing where needed. Wear neoprene gloves during cylinder changeout or wherever contact with product is possible. Select per OSHA 29 CFR 1910.132, 1910.136, and 1910.138.

Respiratory protection : When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure (e.g., an organic vapor cartridge). For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).

Thermal hazard protection : Wear cold insulating gloves when transfilling or breaking transfer connections.

Environmental exposure controls : Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment. Refer to local regulations for restriction of emissions to the atmosphere.

Other information : Consider the use of flame resistant anti-static safety clothing. Wear safety shoes while handling containers. Wear leather safety gloves and safety shoes when handling cylinders.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Gas

Molecular mass : 56 g/mol

Color : Colorless.

Odor : Sweetish.

Odor threshold : Odor threshold is subjective and inadequate to warn for overexposure.

pH	: Not applicable.
Relative evaporation rate (butyl acetate=1)	: No data available
Relative evaporation rate (ether=1)	: Not applicable.
Melting point	: -139 °C
Freezing point	: No data available
Boiling point	: 3.72 °C
Flash point	: Not applicable.
Critical temperature	: 159.9 °C
Auto-ignition temperature	: 325 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: 1.6 - 9.7 vol %
Vapor pressure	: 180 kPa
Critical pressure	: 4197 kPa
Relative vapor density at 20 °C	: No data available
Relative density	: 0.64
Relative gas density	: 2
Solubility	: Water: No data available
Log Pow	: 2.33
Log Kow	: Not applicable.
Viscosity, kinematic	: Not applicable.
Viscosity, dynamic	: Not applicable.
Explosive properties	: Not applicable.
Oxidizing properties	: None.
Explosive limits	: No data available

9.2. Other information

Gas group	: Liquefied gas
Additional information	: Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

May occur. Hazardous polymerization may occur if normal conditions are exceeded. This material is a flammable hydrocarbon and may explode in the presence of oxidizers.

10.4. Conditions to avoid

Catalyst. High temperature. High pressure.

10.5. Incompatible materials

Acids. Halogens. Oxidizing agent.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Skin corrosion/irritation : Not classified
pH: Not applicable.
Serious eye damage/irritation : Not classified
pH: Not applicable.
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
Specific target organ toxicity (single exposure) : Not classified
Specific target organ toxicity (repeated exposure) : Not classified
Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No ecological damage caused by this product.

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

cis-2-Butene (590-18-1)	
Log Pow	2.33
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

12.4. Mobility in soil

cis-2-Butene (590-18-1)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Do not attempt to dispose of residual or unused quantities. Return container to supplier.

SECTION 14: Transport information

In accordance with DOT
Transport document description : UN1075 Petroleum gases, liquefied, 2.1
UN-No.(DOT) : UN1075
Proper Shipping Name (DOT) : Petroleum gases, liquefied
Department of Transportation (DOT) Hazard Classes : 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115
Hazard labels (DOT) : 2.1 - Flammable gas

DOT Special Provisions (49 CFR 172.102)	:	T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

Additional information

Other information	:	No supplementary information available.
Special transport precautions	:	Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers: - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG)	:	1012
Proper Shipping Name (IMDG)	:	PETROLEUM GASES, LIQUEFIED
Class (IMDG)	:	2 - Gases
MFAG-No	:	115

Air transport

UN-No.(IATA)	:	1012
Proper Shipping Name (IATA)	:	Petroleum gases, liquefied
Class (IATA)	:	2
Civil Aeronautics Law	:	Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

cis-2-Butene (590-18-1)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory	
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Sudden release of pressure hazard Fire hazard

15.2. International regulations

CANADA

cis-2-Butene (590-18-1)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

cis-2-Butene (590-18-1)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

15.2.2. National regulations

cis-2-Butene (590-18-1)
Listed on the AICS (Australian Inventory of Chemical Substances) Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China) Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory Listed on the Korean ECL (Existing Chemicals List) Listed on NZIoC (New Zealand Inventory of Chemicals) Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

15.3. US State regulations

cis-2-Butene(590-18-1)	
U.S. - California - Proposition 65 - Carcinogens List	No

cis-2-Butene(590-18-1)	
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

Revision date : 2/20/2015 12:00:00 AM

Other information : When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

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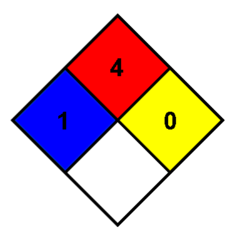
Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc., P.O. Box 44, Tonawanda, NY 14151-0044).

PRAXAIR and the Flowing Airstream design are trademarks or registered trademarks of Praxair Technology, Inc. in the United States and/or other countries.

NFPA health hazard : 1 - Exposure could cause irritation but only minor residual injury even if no treatment is given.

NFPA fire hazard : 4 - Will rapidly or completely vaporize at normal pressure and temperature, or is readily dispersed in air and will burn readily.

NFPA reactivity : 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

Health : 0 Minimal Hazard - No significant risk to health

Flammability : 4 Severe Hazard

Physical : 1 Slight Hazard

1-Butene

Safety Data Sheet P-6214

according to U.S. Code of Federal Regulations 29 CFR 1910.1200, Hazard Communication.

Date of issue: 01/01/1979 Revision date: 02/20/2015 Supersedes: 12/01/2009

SECTION: 1. Product and company identification

1.1. Product identifier

Product form	: Substance
Name	: 1-Butene
CAS No	: 106-98-9
Formula	: C4H8
Other means of identification	: 1-BUTYLENE

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture	: Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
39 Old Ridgebury Road
Danbury, CT 06810-5113 - USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number : Onsite Emergency: 1-800-645-4633

CHEMTREC, 24hr/day 7days/week — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887 (collect calls accepted, Contract 17729)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Gas 1 H220
Liquefied gas H280

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS02 GHS04

Signal word (GHS-US) : DANGER

Hazard statements (GHS-US) :
H220 - EXTREMELY FLAMMABLE GAS
H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED
OSHA-H01 - MAY DISPLACE OXYGEN AND CAUSE RAPID SUFFOCATION.
CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR
CGA-HG01 - MAY CAUSE FROSTBITE.

Precautionary statements (GHS-US) :
P202 - Do not handle until all safety precautions have been read and understood
P210 - Keep away from heat, Open flames, sparks, hot surfaces. - No smoking
P271+P403 - Use and store only outdoors or in a well-ventilated place.
P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely
P381 - Eliminate all ignition sources if safe to do so
CGA-PG05 - Use a back flow preventive device in the piping.
CGA-PG12 - Do not open valve until connected to equipment prepared for use.
CGA-PG06 - Close valve after each use and when empty.
CGA-PG11 - Never put cylinders into unventilated areas of passenger vehicles.
CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

Other hazards not contributing to the classification : None.

2.4. Unknown acute toxicity (GHS-US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%
1-Butene (Main constituent)	(CAS No) 106-98-9	100

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : Immediately remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, qualified personnel may give oxygen. Call a physician.

First-aid measures after skin contact : For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.

First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.

Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.

Reactivity : No reactivity hazard other than the effects described in sub-sections below.

5.3. Advice for firefighters

Firefighting instructions : Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.

Protection during firefighting : Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.

Special protective equipment for fire fighters : Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters.

Specific methods	: Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems. Stop flow of product if safe to do so. Use water spray or fog to knock down fire fumes if possible. Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.
Other information	: Containers are equipped with a pressure relief device. (Exceptions may exist where authorized by DOT.).

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Forms explosive mixtures with air. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling	: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment. This gas is heavier than air and in an enclosed space tends to accumulate near the floor, displacing air and pushing it upward. This creates an oxygen-deficient atmosphere near the floor. Ventilate space before entry. Verify sufficient oxygen concentration. Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post "No Smoking or Open Flames" signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

1-Butene (106-98-9)		
ACGIH	ACGIH TLV-TWA (ppm)	250 ppm
USA OSHA	Not established	

8.2. Exposure controls

Appropriate engineering controls : An explosion-proof local exhaust system is acceptable. Local exhaust and general ventilation must be adequate to meet exposure standards. Mechanic (general) engineering controls: Use only in a closed system. Closed system, ventilation, explosion-proof electrical equipment and lighting.

Eye protection : Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections. Wear safety glasses with side shields.

Skin and body protection : Wear work gloves and metatarsal shoes for cylinder handling. Protective equipment where needed. Select in accordance with OSHA 29 CFR 1910.132, 1910.136, and 1910.138.

Respiratory protection : When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure (e.g., an organic vapor cartridge). For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).

Thermal hazard protection : Wear cold insulating gloves when transfilling or breaking transfer connections.

Environmental exposure controls : Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment. Refer to local regulations for restriction of emissions to the atmosphere.

Other information : Wear safety shoes while handling containers. Consider the use of flame resistant anti-static safety clothing. Wear leather safety gloves and safety shoes when handling cylinders.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Gas

Molecular mass : 56 g/mol

Color : Colorless.

Odor : Sweetish.

Odor threshold : No data available

pH	: Not applicable.
Relative evaporation rate (butyl acetate=1)	: No data available
Relative evaporation rate (ether=1)	: Not applicable.
Melting point	: -185 °C
Freezing point	: No data available
Boiling point	: -6.47 °C (at 760 mmHg)
Flash point	: -80 °C TCC
Critical temperature	: 146.4 °C
Auto-ignition temperature	: 384 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: 1.6 - 9.3 vol %
Vapor pressure	: 260 kPa
Critical pressure	: 4020 kPa
Relative vapor density at 20 °C	: No data available
Relative density	: 0.63
Specific gravity / density	: 0.59 g/cm³ (at 20 °C)
Relative gas density	: 2
Solubility	: Water: No data available
Log Pow	: 2.4
Log Kow	: Not applicable.
Viscosity, kinematic	: Not applicable.
Viscosity, dynamic	: Not applicable.
Explosive properties	: Not applicable.
Oxidizing properties	: None.
Explosive limits	: No data available

9.2. Other information

Gas group	: Liquefied gas
Additional information	: Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

May occur. Hazardous polymerization may occur if normal conditions are exceeded. This material is a flammable hydrocarbon and may explode in the presence of oxidizers.

10.4. Conditions to avoid

High temperature. High pressure. Catalyst.

10.5. Incompatible materials

Oxidizing agent. Acids. Halogens.

10.6. Hazardous decomposition products

Thermal decomposition may produce : Carbon monoxide. Carbon dioxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity	: Not classified

Skin corrosion/irritation : Not classified

pH: Not applicable.

Serious eye damage/irritation : Not classified

pH: Not applicable.

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Reproductive toxicity : Not classified

Specific target organ toxicity (single exposure) : Not classified

Specific target organ toxicity (repeated exposure) : Not classified

Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No ecological damage caused by this product.

12.2. Persistence and degradability

1-Butene (106-98-9)	
Persistence and degradability	Not readily biodegradable.

12.3. Bioaccumulative potential

1-Butene (106-98-9)	
Log Pow	2.4
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

12.4. Mobility in soil

1-Butene (106-98-9)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Do not attempt to dispose of residual or unused quantities. Return container to supplier.

SECTION 14: Transport information

In accordance with DOT

Transport document description : UN1075 Petroleum gases, liquefied, 2.1

UN-No.(DOT) : UN1075

Proper Shipping Name (DOT) : Petroleum gases, liquefied

Department of Transportation (DOT) Hazard Classes : 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115

Hazard labels (DOT)	:	2.1 - Flammable gas 
DOT Special Provisions (49 CFR 172.102)	:	T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

Additional information

Other information	:	No supplementary information available.
Special transport precautions	:	Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers: - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG)	:	1012
Proper Shipping Name (IMDG)	:	PETROLEUM GASES, LIQUEFIED
Class (IMDG)	:	2 - Gases
MFAG-No	:	115

Air transport

UN-No.(IATA)	:	1012
Proper Shipping Name (IATA)	:	Petroleum gases, liquefied
Class (IATA)	:	2
Civil Aeronautics Law	:	Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

1-Butene (106-98-9)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory	
SARA Section 311/312 Hazard Classes	Sudden release of pressure hazard Fire hazard

15.2. International regulations

CANADA

1-Butene (106-98-9)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

1-Butene (106-98-9)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

15.2.2. National regulations

1-Butene (106-98-9)
Listed on the AICS (Australian Inventory of Chemical Substances) Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China) Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory Listed on the Korean ECL (Existing Chemicals List) Listed on NZIoC (New Zealand Inventory of Chemicals) Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

15.3. US State regulations

1-Butene(106-98-9)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

Revision date : 2/20/2015 12:00:00 AM

Other information : When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

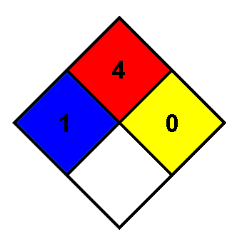
The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc., it is the user's obligation to determine the conditions of safe use of the product.

Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc., P.O. Box 44, Tonawanda, NY 14151-0044).

NFPA health hazard : 1 - Exposure could cause irritation but only minor residual injury even if no treatment is given.

NFPA fire hazard : 4 - Will rapidly or completely vaporize at normal pressure and temperature, or is readily dispersed in air and will burn readily.

NFPA reactivity : 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

Health : 0 Minimal Hazard - No significant risk to health

Flammability : 4 Severe Hazard

Physical : 1 Slight Hazard

SDS US (GHS HazCom 2012) - Praxair

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

1,3-butadiene, buta-1,3-diene

Safety Data Sheet P-4571

according to U.S. Code of Federal Regulations 29 CFR 1910.1200, Hazard Communication.

Date of issue: 01/01/1979 Revision date: 02/20/2015 Supersedes: 05/01/2009

SECTION: 1. Product and company identification

1.1. Product identifier

Product form	:	Substance
Name	:	1,3-butadiene, buta-1,3-diene
CAS No	:	106-99-0
Formula	:	C4H6

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture	:	Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet

Praxair, Inc.
39 Old Ridgebury Road
Danbury, CT 06810-5113 - USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number

Emergency number	:	Onsite Emergency: 1-800-645-4633 CHEMTREC, 24hr/day 7days/week — Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887 (collect calls accepted, Contract 17729)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Gas 1	H220
Liquefied gas	H280
Skin Irrit. 2	H315
Eye Irrit. 2A	H319
Muta. 1B	H340
Carc. 1A	H350

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :

GHS02 GHS04 GHS08

Signal word (GHS-US)	:	DANGER
Hazard statements (GHS-US)	:	H220 - EXTREMELY FLAMMABLE GAS H280 - CONTAINS GAS UNDER PRESSURE; MAY EXPLODE IF HEATED H340 - MAY CAUSE GENETIC DEFECTS H350 - MAY CAUSE CANCER (Inhalation) CGA-HG04 - MAY FORM EXPLOSIVE MIXTURES WITH AIR CGA-HG01 - MAY CAUSE FROSTBITE.
Precautionary statements (GHS-US)	:	P201 - Obtain special instructions before use P202 - Do not handle until all safety precautions have been read and understood P210 - Keep away from heat, Open flames, sparks, hot surfaces. - No smoking P261 - Avoid breathing gas P262 - Do not get in eyes, on skin, or on clothing. P271+P403 - Use and store only outdoors or in a well-ventilated place. P280+P284 - Wear protective gloves, protective clothing, eye protection, respiratory protection, and/or face protection.

P377 - Leaking gas fire: Do not extinguish, unless leak can be stopped safely
P381 - Eliminate all ignition sources if safe to do so
P405 - Store locked up
P501 - Dispose of contents/container in accordance with container supplier/owner instructions
CGA-PG05 - Use a back flow preventive device in the piping.
CGA-PG12 - Do not open valve until connected to equipment prepared for use.
CGA-PG06 - Close valve after each use and when empty.
CGA-PG02 - Protect from sunlight when ambient temperature exceeds 52°C (125°F).

2.3. Other hazards

Other hazards not contributing to the classification : None.

2.4. Unknown acute toxicity (GHS-US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Name	Product identifier	%
1,3-butadiene, buta-1,3-diene (Main constituent)	(CAS No) 106-99-0	100

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures after inhalation : Immediately remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, qualified personnel may give oxygen. Call a physician.

First-aid measures after skin contact : For exposure to liquid, immediately warm frostbite area with warm water not to exceed 105°F (41°C). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.

First-aid measures after ingestion : Ingestion is not considered a potential route of exposure.

4.2. Most important symptoms and effects, both acute and delayed

No additional information available

4.3. Indication of any immediate medical attention and special treatment needed

None. Obtain medical assistance.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Carbon dioxide, Dry chemical, Water spray or fog.

5.2. Special hazards arising from the substance or mixture

Fire hazard : EXTREMELY FLAMMABLE GAS. If venting or leaking gas catches fire, do not extinguish flames. Flammable vapors may spread from leak, creating an explosive reignition hazard. Vapors can be ignited by pilot lights, other flames, smoking, sparks, heaters, electrical equipment, static discharge, or other ignition sources at locations distant from product handling point. Explosive atmospheres may linger. Before entering an area, especially a confined area, check the atmosphere with an appropriate device.

Explosion hazard : EXTREMELY FLAMMABLE GAS. Forms explosive mixtures with air and oxidizing agents.

Reactivity : No reactivity hazard other than the effects described in sub-sections below.

5.3. Advice for firefighters

Firefighting instructions	: Evacuate all personnel from the danger area. Use self-contained breathing apparatus (SCBA) and protective clothing. Immediately cool containers with water from maximum distance. Stop flow of gas if safe to do so, while continuing cooling water spray. Remove ignition sources if safe to do so. Remove containers from area of fire if safe to do so. On-site fire brigades must comply with OSHA 29 CFR 1910.156 and applicable standards under 29 CFR 1910 Subpart L—Fire Protection.
Protection during firefighting	: Compressed gas: asphyxiant. Suffocation hazard by lack of oxygen.
Special protective equipment for fire fighters	: Standard protective clothing and equipment (Self Contained Breathing Apparatus) for fire fighters. Wear gas tight chemically protective clothing in combination with self contained breathing apparatus.
Specific methods	: Use fire control measures appropriate for the surrounding fire. Exposure to fire and heat radiation may cause gas containers to rupture. Cool endangered containers with water spray jet from a protected position. Prevent water used in emergency cases from entering sewers and drainage systems. Stop flow of product if safe to do so. Use water spray or fog to knock down fire fumes if possible. Do not extinguish a leaking gas flame unless absolutely necessary. Spontaneous/explosive re-ignition may occur. Extinguish any other fire.
Other information	: Containers are equipped with a pressure relief device. (Exceptions may exist where authorized by DOT.).

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Forms explosive mixtures with air. Immediately evacuate all personnel from danger area. Use self-contained breathing apparatus where needed. Remove all sources of ignition if safe to do so. Reduce vapors with fog or fine water spray, taking care not to spread liquid with water. Shut off flow if safe to do so. Ventilate area or move container to a well-ventilated area. Flammable vapors may spread from leak and could explode if reignited by sparks or flames. Explosive atmospheres may linger. Before entering area, especially confined areas, check atmosphere with an appropriate device.

6.1.1. For non-emergency personnel

No additional information available

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Try to stop release. Reduce vapor with fog or fine water spray. Prevent waste from contaminating the surrounding environment. Prevent soil and water pollution. Dispose of contents/container in accordance with local/regional/national/international regulations. Contact supplier for any special requirements.

6.3. Methods and material for containment and cleaning up

No additional information available

6.4. Reference to other sections

See also sections 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Use only non-sparking tools. Use only explosion-proof equipment.

Ensure equipment is adequately grounded.

Leak-check system with soapy water; never use a flame.

Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store only where temperature will not exceed 125°F (52°C). Post “No Smoking or Open Flames” signs in storage and use areas. There must be no sources of ignition. Separate packages and protect against potential fire and/or explosion damage following appropriate codes and requirements (e.g., NFPA 30, NFPA 55, NFPA 70, and/or NFPA 221 in the U.S.) or according to requirements determined by the Authority Having Jurisdiction (AHJ). Always secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand when the container is not in use. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods. For other precautions in using this product, see section 16.

OTHER PRECAUTIONS FOR HANDLING, STORAGE, AND USE: When handling product under pressure, use piping and equipment adequately designed to withstand the pressures to be encountered. Never work on a pressurized system. Use a back flow preventive device in the piping. Gases can cause rapid suffocation because of oxygen deficiency; store and use with adequate ventilation. If a leak occurs, close the container valve and blow down the system in a safe and environmentally correct manner in compliance with all international, federal/national, state/provincial, and local laws; then repair the leak. Never place a container where it may become part of an electrical circuit.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

1,3-butadiene, buta-1,3-diene (106-99-0)		
ACGIH	ACGIH TLV-TWA (ppm)	2 ppm
USA OSHA	OSHA PEL (TWA) (ppm)	1 ppm
USA OSHA	OSHA PEL (STEL) (ppm)	5 ppm (see 29 CFR 1910.1051)

8.2. Exposure controls

Appropriate engineering controls : This product must be confined with vapor-tight equipment. With this confinement, vapors should not be released, and local exhaust should be satisfactory. An explosion-proof system is acceptable. Ensure that any venting of material is in compliance with international, federal/national, state/provincial, and local regulations.

Hand protection : Wear protective gloves made of PVC.

Eye protection : Wear safety glasses with side shields. Wear safety glasses with side shields or goggles when transfilling or breaking transfer connections. Provide readily accessible eye wash stations and safety showers.

Skin and body protection	: Wear work gloves and metatarsal shoes for cylinder handling. Protective equipment where needed. Select in accordance with OSHA 29 CFR 1910.132, 1910.136, and 1910.138.
Respiratory protection	: When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure (e.g., an organic vapor cartridge). For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).
Environmental exposure controls	: Refer to local regulations for restriction of emissions to the atmosphere. See section 13 for specific methods for waste gas treatment. Refer to local regulations for restriction of emissions to the atmosphere.
Other information	: Consider the use of flame resistant anti-static safety clothing. Wear safety shoes while handling containers. Keep suitable chemically resistant protective clothing readily available for emergency use. Wear leather safety gloves and safety shoes when handling cylinders.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Gas
Appearance	: Gas or low boiling-point liquid.
Molecular mass	: 54 g/mol
Color	: Colorless.
Odor	: Mildly aromatic.
Odor threshold	: Odor threshold is subjective and inadequate to warn for overexposure. 1 mg/m³ (Hellman and Small)
pH	: Not applicable.
Relative evaporation rate (butyl acetate=1)	: > 25
Relative evaporation rate (ether=1)	: Not applicable.
Melting point	: -109 °C
Freezing point	: No data available
Boiling point	: -4.419 °C
Flash point	: -76.1 °C (TCC ASTM D56)
Critical temperature	: 151.9 °C
Auto-ignition temperature	: 418.9 °C
Decomposition temperature	: No data available
Flammability (solid, gas)	: 2 - 11.5 vol %
Vapor pressure	: 240 kPa
Critical pressure	: 4330 kPa
Relative vapor density at 20 °C	: No data available
Relative density	: 0.65
Specific gravity / density	: 0.6149 g/cm³ (at 25 °C)
Relative gas density	: 1.9
Solubility	: Water: 1025 mg/l
Log Pow	: 1.99
Log Kow	: Not applicable.
Viscosity, kinematic	: Not applicable.
Viscosity, dynamic	: Not applicable.
Explosive properties	: Not applicable.
Oxidizing properties	: None.
Explosive limits	: No data available

9.2. Other information

Gas group	: Liquefied gas

Additional information : Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

SECTION 10: Stability and reactivity

10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

10.2. Chemical stability

May polymerise. Inhibitor usually added. Stable under normal conditions.

10.3. Possibility of hazardous reactions

May occur. May react violently with oxidants. Can form explosive mixture with air.

10.4. Conditions to avoid

Keep away from heat/sparks/open flames/hot surfaces. – No smoking. Rusty iron. Exposure to air may form spontaneously flammable or explosive peroxides.

10.5. Incompatible materials

Oxidizing agent. Acids. Halogens. Sulphur dioxide. Phenol. Protopaldehyde.

10.6. Hazardous decomposition products

Thermal decomposition may produce : Carbon monoxide. Carbon dioxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

1,3-butadiene, buta-1,3-diene (\f)106-99-0	
LD50 oral rat	5480 mg/kg
LC50 inhalation rat (mg/l)	285 g/m³ (Exposure time: 4 h)
ATE US (oral)	5480.000 mg/kg body weight
ATE US (vapors)	285.000 mg/l/4h
ATE US (dust, mist)	285.000 mg/l/4h

Skin corrosion/irritation : CAUSES SKIN IRRITATION.
pH: Not applicable.
Serious eye damage/irritation : CAUSES SERIOUS EYE IRRITATION.
pH: Not applicable.
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : MAY CAUSE GENETIC DEFECTS.
Carcinogenicity : MAY CAUSE CANCER (Inhalation).

1,3-butadiene, buta-1,3-diene (106-99-0)	
IARC group	1 - Carcinogenic to humans
National Toxicology Program (NTP) Status	1 - Evidence of Carcinogenicity, 2 - Known Human Carcinogens

Reproductive toxicity : Not classified
Specific target organ toxicity (single exposure) : Not classified
Specific target organ toxicity (repeated exposure) : Not classified
Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : No ecological damage caused by this product.

12.2. Persistence and degradability

1,3-butadiene, buta-1,3-diene (106-99-0)	
Persistence and degradability	Not readily biodegradable.

12.3. Bioaccumulative potential

1,3-butadiene, buta-1,3-diene (106-99-0)	
BCF fish 1	13 - 19.1
Log Pow	1.99
Log Kow	Not applicable.
Bioaccumulative potential	Not expected to bioaccumulate due to the low log Kow (log Kow < 4). Refer to section 9.

12.4. Mobility in soil

1,3-butadiene, buta-1,3-diene (106-99-0)	
Mobility in soil	No data available.
Ecology - soil	Because of its high volatility, the product is unlikely to cause ground or water pollution.

12.5. Other adverse effects

Other adverse effects : May cause pH changes in aqueous ecological systems.

Effect on ozone layer : None.

Effect on the global warming : No known effects from this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Do not attempt to dispose of residual or unused quantities. Return container to supplier.

SECTION 14: Transport information

In accordance with DOT

Transport document description : UN1010 Butadienes, stabilized, 2.1

UN-No.(DOT) : UN1010

Proper Shipping Name (DOT) : Butadienes, stabilized

Department of Transportation (DOT) Hazard Classes : 2.1 - Class 2.1 - Flammable gas 49 CFR 173.115

Hazard labels (DOT) : 2.1 - Flammable gas

DOT Special Provisions (49 CFR 172.102) : T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

Additional information

Other information : No supplementary information available.

Special transport precautions : Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers: - Ensure there is adequate ventilation. - Ensure that containers are firmly secured. - Ensure cylinder valve is closed and not leaking. - Ensure valve outlet cap nut or plug (where provided) is correctly fitted. - Ensure valve protection device (where provided) is correctly fitted.

Transport by sea

UN-No. (IMDG) : 1010

Proper Shipping Name (IMDG) : BUTADIENES, STABILIZED

Class (IMDG)	:	2 - Gases
MFAG-No	:	116P

Air transport

UN-No.(IATA)	:	1010
Proper Shipping Name (IATA)	:	Butadienes, stabilized
Class (IATA)	:	2
Civil Aeronautics Law	:	Gases under pressure/Gases flammable under pressure

SECTION 15: Regulatory information

15.1. US Federal regulations

1,3-butadiene, buta-1,3-diene (106-99-0)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory Listed on United States SARA Section 313	
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard Sudden release of pressure hazard Reactive hazard Fire hazard
SARA Section 313 - Emission Reporting	0.1 %

15.2. International regulations

CANADA

1,3-butadiene, buta-1,3-diene (106-99-0)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

1,3-butadiene, buta-1,3-diene (106-99-0)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

15.2.2. National regulations

1,3-butadiene, buta-1,3-diene (106-99-0)
Listed on IARC (International Agency for Research on Cancer) Listed on the AICS (Australian Inventory of Chemical Substances) Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China) Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory Listed on the Korean ECL (Existing Chemicals List) Listed on NZIoC (New Zealand Inventory of Chemicals) Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances) Japanese Pollutant Release and Transfer Register Law (PRTR Law) Listed as carcinogen on NTP (National Toxicology Program) Listed on the Canadian IDL (Ingredient Disclosure List)

15.3. US State regulations

1,3-butadiene, buta-1,3-diene(106-99-0)	
U.S. - California - Proposition 65 - Carcinogens List	Yes
U.S. - California - Proposition 65 - Developmental Toxicity	Yes
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	Yes
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
No significance risk level (NSRL)	0.4 µg/day
State or local regulations	U.S. - Massachusetts - Right To Know List

1,3-butadiene, buta-1,3-diene(106-99-0)	
	U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List U.S. - Pennsylvania - RTK (Right to Know) - Special Hazardous Substances U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

Revision date : 2/20/2015 12:00:00 AM

Other information : Prior to using any plastics, confirm their compatibility with this chemical.

When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc., it is the user's obligation to determine the conditions of safe use of the product.

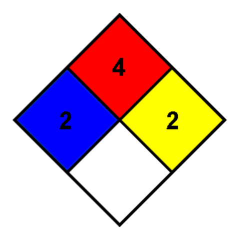
Praxair SDSs are furnished on sale or delivery by Praxair or the independent distributors and suppliers who package and sell our products. To obtain current SDSs for these products, contact your Praxair sales representative, local distributor, or supplier, or download from www.praxair.com. If you have questions regarding Praxair SDSs, would like the document number and date of the latest SDS, or would like the names of the Praxair suppliers in your area, phone or write the Praxair Call Center (Phone: 1-800-PRAXAIR/1-800-772-9247; Address: Praxair Call Center, Praxair, Inc., P.O. Box 44, Tonawanda, NY 14151-0044).

PRAXAIR and the Flowing Airstream design are trademarks or registered trademarks of Praxair Technology, Inc. in the United States and/or other countries.

NFPA health hazard : 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.

NFPA fire hazard : 4 - Will rapidly or completely vaporize at normal pressure and temperature, or is readily dispersed in air and will burn readily.

NFPA reactivity : 2 - Normally unstable and readily undergo violent decomposition but do not detonate. Also: may react violently with water or may form potentially explosive mixtures with water.



HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 4 Severe Hazard

Physical : 2 Moderate Hazard

SDS US (GHS HazCom 2012) - Praxair

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

MATERIAL SAFETY DATA SHEET

1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

MATHESON TRI-GAS, INC.
150 Allen Road Suite 302
Basking Ridge, New Jersey 07920
Information: 1-800-416-2505

Emergency Contact:
CHEMTREC 1-800-424-9300
Calls Originating Outside the US:
703-527-3887 (Collect Calls Accepted)

SUBSTANCE: CIS-2-PENTENE

TRADE NAMES/SYNONYMS:
MTG MSDS 175; 2-PENTENE, (Z)-; CIS-BETA-AMYLENE; CIS-PENTENE; (Z)-2-PENTENE; PENTENE; CIS-METHYLETHYLETHYLENE; 2-PENTENE; 2-PENTENE(CIS); C5H10; MAT18214

CHEMICAL FAMILY: hydrocarbons, aliphatic

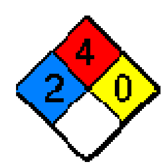
CREATION DATE: Mar 02 1989
REVISION DATE: Dec 11 2008

2. COMPOSITION, INFORMATION ON INGREDIENTS

COMPONENT: CIS-2-PENTENE
CAS NUMBER: 627-20-3
PERCENTAGE: 100.0

3. HAZARDS IDENTIFICATION

NFPA RATINGS (SCALE 0-4): HEALTH=2 FIRE=4 REACTIVITY=0



EMERGENCY OVERVIEW:
COLOR: colorless
PHYSICAL FORM: liquid
MAJOR HEALTH HAZARDS: skin irritation, eye irritation
PHYSICAL HAZARDS: Flammable liquid and vapor. Vapor may cause flash fire.

POTENTIAL HEALTH EFFECTS:
INHALATION:
SHORT TERM EXPOSURE: irritation, nausea, vomiting, symptoms of drunkenness, convulsions, coma
LONG TERM EXPOSURE: no information is available
SKIN CONTACT:

SHORT TERM EXPOSURE: irritation
LONG TERM EXPOSURE: same as effects reported in short term exposure
EYE CONTACT:
SHORT TERM EXPOSURE: irritation
LONG TERM EXPOSURE: same as effects reported in short term exposure
INGESTION:
SHORT TERM EXPOSURE: nausea, stomach pain, symptoms of drunkenness
LONG TERM EXPOSURE: no information is available

4. FIRST AID MEASURES

INHALATION: If adverse effects occur, remove to uncontaminated area. Give artificial respiration if not breathing. Get immediate medical attention.

SKIN CONTACT: Wash skin with soap and water for at least 15 minutes while removing contaminated clothing and shoes. Get medical attention, if needed. Thoroughly clean and dry contaminated clothing and shoes before reuse.

EYE CONTACT: Flush eyes with plenty of water for at least 15 minutes. Then get immediate medical attention.

INGESTION: Get medical attention immediately.

NOTE TO PHYSICIAN: For ingestion, consider gastric lavage.

5. FIRE FIGHTING MEASURES

FIRE AND EXPLOSION HAZARDS: Severe fire hazard. The vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. Vapor/air mixtures are explosive.

EXTINGUISHING MEDIA: regular dry chemical, carbon dioxide, water, regular foam

Large fires: Use regular foam or flood with fine water spray.

FIRE FIGHTING: Move container from fire area if it can be done without risk. Cool containers with water spray until well after the fire is out. Stay away from the ends of tanks. For fires in cargo or storage area: Cool containers with water from unmanned hose holder or monitor nozzles until well after fire is out. If this is impossible then take the following precautions: Keep unnecessary people away, isolate hazard area and deny entry. Let the fire burn. Withdraw immediately in case of rising sound from venting safety device or any discoloration of tanks due to fire. For tank, rail car or tank truck: Evacuation radius: 800 meters (1/2 mile). Do not attempt to extinguish fire unless flow of material can be stopped first. Flood with fine water spray. Do not scatter spilled material with high-pressure water streams. Cool containers with water spray until well after the fire is out. Apply water from a protected location or from a safe distance. Avoid inhalation of material or combustion by-products. Stay upwind and keep out of low areas.

FLASH POINT: <-4 F (<-20 C) (CC)
FLAMMABILITY CLASS (OSHA): IA

6. ACCIDENTAL RELEASE MEASURES

OCCUPATIONAL RELEASE:
Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk. Reduce vapors with water spray. Small spills: Absorb with sand or other non-combustible material. Collect spilled material in appropriate container for disposal. Large spills: Dike for later disposal. Remove sources of ignition. Keep unnecessary people away, isolate hazard area and deny entry.

7. HANDLING AND STORAGE

STORAGE: Store and handle in accordance with all current regulations and standards. Subject to storage regulations: U.S. OSHA 29 CFR 1910.106. Grounding and bonding required. Keep separated from incompatible substances.

8. EXPOSURE CONTROLS, PERSONAL PROTECTION

EXPOSURE LIMITS:
CIS-2-PENTENE:
No occupational exposure limits established.

VENTILATION: Provide local exhaust ventilation system. Ventilation equipment should be explosion-resistant if explosive concentrations of material are present. Ensure compliance with applicable exposure limits.

EYE PROTECTION: Wear splash resistant safety goggles. Provide an emergency eye wash fountain and quick drench shower in the immediate work area.

CLOTHING: Wear appropriate chemical resistant clothing.

GLOVES: Wear appropriate chemical resistant gloves.

RESPIRATOR: Under conditions of frequent use or heavy exposure, respiratory protection may be needed. Respiratory protection is ranked in order from minimum to maximum. Consider warning properties before use.
Any chemical cartridge respirator with organic vapor cartridge(s).
Any chemical cartridge respirator with a full facepiece and organic vapor cartridge(s).
Any air-purifying respirator with a full facepiece and an organic vapor canister.
For Unknown Concentrations or Immediately Dangerous to Life or Health -
Any supplied-air respirator with a full facepiece that is operated in a pressure-demand or other positive-

pressure mode in combination with an auxiliary self-contained breathing apparatus operated in pressure-demand or other positive-pressure mode.
Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode.

9. PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE: liquid
COLOR: colorless
ODOR: Not available
MOLECULAR WEIGHT: 70.13
MOLECULAR FORMULA: C-H3-C-H2-C-H-C-H-C-H3
BOILING POINT: 99 F (37 C)
FREEZING POINT: -240 F (-151 C)
VAPOR PRESSURE: 426 mmHg @ 21 C
VAPOR DENSITY (air=1): 2.42
SPECIFIC GRAVITY (water=1): 0.6556
WATER SOLUBILITY: insoluble
PH: Not available
VOLATILITY: Not available
ODOR THRESHOLD: Not available
EVAPORATION RATE: Not available
COEFFICIENT OF WATER/OIL DISTRIBUTION: Not available
SOLVENT SOLUBILITY:
Soluble: alcohol, ether, benzene

10. STABILITY AND REACTIVITY

REACTIVITY: Stable at normal temperatures and pressure.

CONDITIONS TO AVOID: Avoid heat, flames, sparks and other sources of ignition. Containers may rupture or explode if exposed to heat. Keep out of water supplies and sewers.

INCOMPATIBILITIES: oxidizing materials, halogens, acids

HAZARDOUS DECOMPOSITION:
Thermal decomposition products: oxides of carbon

POLYMERIZATION: Will not polymerize.

11. TOXICOLOGICAL INFORMATION

CIS-2-PENTENE:
LOCAL EFFECTS:
Irritant: skin, eye

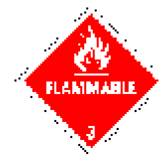
12. ECOLOGICAL INFORMATION

Not available

13. DISPOSAL CONSIDERATIONS

Subject to disposal regulations: U.S. EPA 40 CFR 262. Hazardous Waste Number(s): D001. Dispose in accordance with all applicable regulations.

14. TRANSPORT INFORMATION



U.S. DOT 49 CFR 172.101:
PROPER SHIPPING NAME: Flammable liquids, n.o.s. (CIS-2-PENTENE)
ID NUMBER: UN1993
HAZARD CLASS OR DIVISION: 3
PACKING GROUP: I
LABELING REQUIREMENTS: 3

CANADIAN TRANSPORTATION OF DANGEROUS GOODS:
SHIPPING NAME: Flammable liquid, n.o.s. (CIS-2-PENTENE)
UN NUMBER: UN1993
CLASS: 3
PACKING GROUP/CATEGORY: I

15. REGULATORY INFORMATION

U.S. REGULATIONS:
CERCLA SECTIONS 102a/103 HAZARDOUS SUBSTANCES (40 CFR 302.4): Not regulated.

SARA TITLE III SECTION 302 EXTREMELY HAZARDOUS SUBSTANCES (40 CFR 355 Subpart B): Not regulated.

SARA TITLE III SECTION 304 EXTREMELY HAZARDOUS SUBSTANCES (40 CFR 355 Subpart C): Not regulated.

SARA TITLE III SARA SECTIONS 311/312 HAZARDOUS CATEGORIES (40 CFR 370 Subparts B and C):
ACUTE: Yes

CHRONIC: No
FIRE: Yes
REACTIVE: No
SUDDEN RELEASE: No

SARA TITLE III SECTION 313 (40 CFR 372.65): Not regulated.

OSHA PROCESS SAFETY (29 CFR 1910.119): Not regulated.

STATE REGULATIONS:
California Proposition 65: Not regulated.

CANADIAN REGULATIONS:
WHMIS CLASSIFICATION: B

NATIONAL INVENTORY STATUS:
U.S. INVENTORY (TSCA): Listed on inventory.

TSCA 12(b) EXPORT NOTIFICATION: Not listed.

CANADA INVENTORY (DSL/NDSL): Not determined.

16. OTHER INFORMATION

MATHESON TRI-GAS, INC. MAKES NO EXPRESS OR IMPLIED WARRANTIES, GUARANTEES OR REPRESENTATIONS REGARDING THE PRODUCT OR THE INFORMATION HEREIN, INCLUDING BUT NOT LIMITED TO ANY IMPLIED WARRANTY OF MERCHANTABILITY OR FITNESS FOR USE. MATHESON TRI-GAS, INC. SHALL NOT BE LIABLE FOR ANY PERSONAL INJURY, PROPERTY OR OTHER DAMAGES OF ANY NATURE, WHETHER COMPENSATORY, CONSEQUENTIAL, EXEMPLARY, OR OTHERWISE, RESULTING FROM ANY PUBLICATION, USE OR RELIANCE UPON THE INFORMATION HEREIN.

MATERIAL SAFETY DATA SHEET

1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

MATHESON TRI-GAS, INC.
150 Allen Road Suite 302
Basking Ridge, New Jersey 07920
Information: 1-800-416-2505

Emergency Contact:
CHEMTREC 1-800-424-9300
Calls Originating Outside the US:
703-527-3887 (Collect Calls Accepted)

SUBSTANCE: TRANS-2-PENTENE

TRADE NAMES/SYNONYMS:
MTG MSDS 198; 2-PENTENE; TRANS-BETA-AMYLENE; 2-PENTENE, (E)-; (E)-2-PENTENE; 2-AMYLENE; C5H10; MAT23707

CHEMICAL FAMILY: hydrocarbons, aliphatic

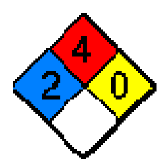
CREATION DATE: Mar 02 1989
REVISION DATE: Dec 11 2008

2. COMPOSITION, INFORMATION ON INGREDIENTS

COMPONENT: TRANS-2-PENTENE
CAS NUMBER: 646-04-8
PERCENTAGE: 100.0

3. HAZARDS IDENTIFICATION

NFPA RATINGS (SCALE 0-4): HEALTH=2 FIRE=4 REACTIVITY=0



EMERGENCY OVERVIEW:
PHYSICAL FORM: liquid
MAJOR HEALTH HAZARDS: skin irritation, eye irritation
PHYSICAL HAZARDS: Flammable liquid and vapor. Vapor may cause flash fire.

POTENTIAL HEALTH EFFECTS:
INHALATION:
SHORT TERM EXPOSURE: irritation, nausea, vomiting, symptoms of drunkenness, convulsions, coma
LONG TERM EXPOSURE: no information is available
SKIN CONTACT:
SHORT TERM EXPOSURE: irritation

LONG TERM EXPOSURE: same as effects reported in short term exposure
EYE CONTACT:
SHORT TERM EXPOSURE: irritation
LONG TERM EXPOSURE: same as effects reported in short term exposure
INGESTION:
SHORT TERM EXPOSURE: nausea, stomach pain, symptoms of drunkenness
LONG TERM EXPOSURE: no information is available

4. FIRST AID MEASURES

INHALATION: If adverse effects occur, remove to uncontaminated area. Give artificial respiration if not breathing. Get immediate medical attention.

SKIN CONTACT: Wash skin with soap and water for at least 15 minutes while removing contaminated clothing and shoes. Get medical attention, if needed. Thoroughly clean and dry contaminated clothing and shoes before reuse.

EYE CONTACT: Flush eyes with plenty of water for at least 15 minutes. Then get immediate medical attention.

INGESTION: Get medical attention immediately.

NOTE TO PHYSICIAN: For ingestion, consider gastric lavage.

5. FIRE FIGHTING MEASURES

FIRE AND EXPLOSION HAZARDS: Severe fire hazard. The vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. Vapor/air mixtures are explosive.

EXTINGUISHING MEDIA: regular dry chemical, carbon dioxide, water, regular foam

Large fires: Use regular foam or flood with fine water spray.

FIRE FIGHTING: Move container from fire area if it can be done without risk. Cool containers with water spray until well after the fire is out. Stay away from the ends of tanks. For fires in cargo or storage area: Cool containers with water from unmanned hose holder or monitor nozzles until well after fire is out. If this is impossible then take the following precautions: Keep unnecessary people away, isolate hazard area and deny entry. Let the fire burn. Withdraw immediately in case of rising sound from venting safety device or any discoloration of tanks due to fire. For tank, rail car or tank truck: Evacuation radius: 800 meters (1/2 mile). Do not attempt to extinguish fire unless flow of material can be stopped first. Flood with fine water spray. Do not scatter spilled material with high-pressure water streams. Cool containers with water spray until well after the fire is out. Apply water from a protected location or from a safe distance. Avoid inhalation of material or combustion by-products. Stay upwind and keep out of low areas.

FLASH POINT: -49 F (-45 C)
FLAMMABILITY CLASS (OSHA): IA

6. ACCIDENTAL RELEASE MEASURES

OCCUPATIONAL RELEASE:
Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk. Reduce vapors with water spray. Small spills: Absorb with sand or other non-combustible material. Collect spilled material in appropriate container for disposal. Large spills: Dike for later disposal. Remove sources of ignition. Keep unnecessary people away, isolate hazard area and deny entry.

7. HANDLING AND STORAGE

STORAGE: Store and handle in accordance with all current regulations and standards. Subject to storage regulations: U.S. OSHA 29 CFR 1910.106. Grounding and bonding required. Keep separated from incompatible substances.

8. EXPOSURE CONTROLS, PERSONAL PROTECTION

EXPOSURE LIMITS:
TRANS-2-PENTENE:
No occupational exposure limits established.

VENTILATION: Provide local exhaust ventilation system. Ventilation equipment should be explosion-resistant if explosive concentrations of material are present. Ensure compliance with applicable exposure limits.

EYE PROTECTION: Wear splash resistant safety goggles. Provide an emergency eye wash fountain and quick drench shower in the immediate work area.

CLOTHING: Wear appropriate chemical resistant clothing.

GLOVES: Wear appropriate chemical resistant gloves.

RESPIRATOR: Under conditions of frequent use or heavy exposure, respiratory protection may be needed. Respiratory protection is ranked in order from minimum to maximum. Consider warning properties before use.
Any chemical cartridge respirator with organic vapor cartridge(s).
Any chemical cartridge respirator with a full facepiece and organic vapor cartridge(s).
Any air-purifying respirator with a full facepiece and an organic vapor canister.
For Unknown Concentrations or Immediately Dangerous to Life or Health -
Any supplied-air respirator with a full facepiece that is operated in a pressure-demand or other positive-pressure mode in combination with an auxiliary self-contained breathing apparatus operated in pressure-

demand or other positive-pressure mode.
Any self-contained breathing apparatus that has a full facepiece and is operated in a pressure-demand or other positive-pressure mode.

9. PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE: liquid
ODOR: Not available
MOLECULAR WEIGHT: 70.13
MOLECULAR FORMULA: C-H3-C-H2-C-H-C-H-C-H3
BOILING POINT: 97 F (36 C)
FREEZING POINT: -213 F (-136 C)
VAPOR PRESSURE: Not available
VAPOR DENSITY (air=1): 2.42
SPECIFIC GRAVITY (water=1): 0.6482
WATER SOLUBILITY: insoluble
PH: Not available
VOLATILITY: Not available
ODOR THRESHOLD: Not available
EVAPORATION RATE: Not available
COEFFICIENT OF WATER/OIL DISTRIBUTION: Not available
SOLVENT SOLUBILITY:
Soluble: alcohol, ether, benzene

10. STABILITY AND REACTIVITY

REACTIVITY: Stable at normal temperatures and pressure.

CONDITIONS TO AVOID: Avoid heat, flames, sparks and other sources of ignition. Containers may rupture or explode if exposed to heat. Keep out of water supplies and sewers.

INCOMPATIBILITIES: oxidizing materials, halogens, acids

HAZARDOUS DECOMPOSITION:
Thermal decomposition products: oxides of carbon

POLYMERIZATION: Will not polymerize.

11. TOXICOLOGICAL INFORMATION

TRANS-2-PENTENE:
LOCAL EFFECTS:
Irritant: skin, eye

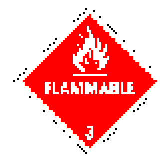
12. ECOLOGICAL INFORMATION

Not available

13. DISPOSAL CONSIDERATIONS

Subject to disposal regulations: U.S. EPA 40 CFR 262. Hazardous Waste Number(s): D001. Dispose in accordance with all applicable regulations.

14. TRANSPORT INFORMATION



U.S. DOT 49 CFR 172.101:
PROPER SHIPPING NAME: Flammable liquids, n.o.s. (trans-2-pentene)
ID NUMBER: UN1993
HAZARD CLASS OR DIVISION: 3
PACKING GROUP: II
LABELING REQUIREMENTS: 3

CANADIAN TRANSPORTATION OF DANGEROUS GOODS:
SHIPPING NAME: Flammable liquid, n.o.s. (TRANS-2-PENTENE)
UN NUMBER: UN1993
CLASS: 3
PACKING GROUP/CATEGORY: II

15. REGULATORY INFORMATION

U.S. REGULATIONS:
CERCLA SECTIONS 102a/103 HAZARDOUS SUBSTANCES (40 CFR 302.4): Not regulated.

SARA TITLE III SECTION 302 EXTREMELY HAZARDOUS SUBSTANCES (40 CFR 355 Subpart B): Not regulated.

SARA TITLE III SECTION 304 EXTREMELY HAZARDOUS SUBSTANCES (40 CFR 355 Subpart C): Not regulated.

SARA TITLE III SARA SECTIONS 311/312 HAZARDOUS CATEGORIES (40 CFR 370 Subparts B and C):
ACUTE: Yes
CHRONIC: No
FIRE: Yes
REACTIVE: No

SUDDEN RELEASE: No

SARA TITLE III SECTION 313 (40 CFR 372.65): Not regulated.

OSHA PROCESS SAFETY (29 CFR 1910.119): Not regulated.

STATE REGULATIONS:
California Proposition 65: Not regulated.

CANADIAN REGULATIONS:
WHMIS CLASSIFICATION: B

NATIONAL INVENTORY STATUS:
U.S. INVENTORY (TSCA): Listed on inventory.

TSCA 12(b) EXPORT NOTIFICATION: Not listed.

CANADA INVENTORY (DSL/NDSL): Not determined.

16. OTHER INFORMATION

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SAFETY DATA SHEET

Revision Date 10-Feb-2015 **Revision Number** 1

1. Identification

Product Name	**cis-3-Hexene**
Cat No. :	**AC379630000; AC379630010; AC379630050**
Synonyms	None Known.
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Entity / Business Name
Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number
For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No.**US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2

Label Elements

Signal Word
Danger

Hazard Statements
Highly flammable liquid and vapor

Precautionary Statements
Prevention
Keep away from heat/sparks/open flames/hot surfaces. - No smoking

Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting/equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Wear protective gloves/protective clothing/eye protection/face protection

Skin
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

Fire
In case of fire: Use CO2, dry chemical, or foam for extinction

Storage
Store in a well-ventilated place. Keep cool

Disposal
Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)
None identified

Unknown Acute Toxicity
.? % of the mixture consists of ingredients of unknown toxicity.

3. Composition / information on ingredients

Component	CAS-No	Weight %
3-Hexene, (Z)-	7642-09-3	97

4. First-aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Obtain medical attention.

Skin Contact Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Obtain medical attention.

Inhalation Remove from exposure, lie down. Move to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Obtain medical attention.

Ingestion Clean mouth with water. Get medical attention.

Most important symptoms/effects Breathing difficulties. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray. Carbon dioxide (CO_2). Dry chemical. chemical foam.

Unsuitable Extinguishing Media No information available

Flash Point -12 °C / 10.4 °F
Method - No information available

Autoignition Temperature No information available
Explosion Limits
Upper No data available
Lower No data available
Sensitivity to Mechanical Impact No information available
Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Flammable.

Hazardous Combustion Products
Carbon monoxide (CO) Carbon dioxide (CO_2)
Protective Equipment and Precautions for Firefighters
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
0	3	0	N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment.
Environmental Precautions	See Section 12 for additional ecological information.
Methods for Containment and Clean Up	Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling	Avoid contact with skin and eyes. Do not breathe dust. Do not breathe vapors or spray mist. Use explosion-proof equipment. Use only non-sparking tools.
Storage	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat and sources of ignition. Flammables area.

8. Exposure controls / personal protection

Exposure Guidelines	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
Engineering Measures	Ensure adequate ventilation, especially in confined areas.

Personal Protective Equipment

Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Clear
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	67 °C / 152.6 °F @ 760 mmHg
Flash Point	-12 °C / 10.4 °F

Evaporation Rate	No information available
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	No information available
Relative Density	0.677
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C6 H12
Molecular Weight	84.16

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable.

Conditions to Avoid Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.

Incompatible Materials Acids, Bases

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information	No acute toxicity information is available for this product
Oral LD50	Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Dermal LD50	Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Vapor LC50	Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.
Component Information	
Toxicologically Synergistic Products	No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
3-Hexene, (Z)-	7642-09-3	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure	None known
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects,both acute and delayed	Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability	No information available
Bioaccumulation/ Accumulation	No information available.
Mobility	No information available.

13. Disposal considerations

Waste Disposal Methods	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No	UN3295
Hazard Class	3
Packing Group	II

TDG

UN-No	UN3295
Hazard Class	3
Packing Group	II

IATA

UN-No	3295
Proper Shipping Name	HYDROCARBONS, LIQUID, N.O.S.
Hazard Class	3
Packing Group	II

IMDG/IMO

UN-No	3295
Proper Shipping Name	HYDROCARBONS, LIQUID, N.O.S.
Hazard Class	3
Packing Group	II

15. Regulatory information

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
3-Hexene, (Z)-	-	-	-	-	-		-	X	-	-	-

Legend:
X - Listed
E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.
F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.
N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.
P - Indicates a commenced PMN substance
R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.
S - Indicates a substance that is identified in a proposed or final Significant New Use Rule

T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.
XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B).
Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.
Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b)	Not applicable
SARA 313	Not applicable

SARA 311/312 Hazardous Categorization

Acute Health Hazard	No
Chronic Health Hazard	No
Fire Hazard	Yes
Sudden Release of Pressure Hazard	No
Reactive Hazard	No

Clean Water Act	Not applicable
Clean Air Act	Not applicable

OSHA Occupational Safety and Health Administration
Not applicable

CERCLA
Not applicable

California Proposition 65	This product does not contain any Proposition 65 chemicals
State Right-to-Know	Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security
This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Canada
This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all the information required by the CPR

WHMIS Hazard Class B2 Flammable liquid

16. Other information

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Revision Date	10-Feb-2015
Print Date	10-Feb-2015
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS)

Disclaimer

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

End of SDS

SAFETY DATA SHEET

Creation Date 27-Sep-2014 **Revision Date** 27-Jan-2015 **Revision Number** 1

1. Identification

Product Name **trans-3-Hexene**

Cat No. : **AC149910000; AC149910010; AC149910050; AC149910051; AC149910250**

Synonyms trans-Hex-3-ene

Recommended Use Laboratory chemicals.

Uses advised against No Information available

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Entity / Business Name
Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number
For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No.**US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Acute oral toxicity	Category 4
Aspiration Toxicity	Category 1

Label Elements

Signal Word
Danger

Hazard Statements
Highly flammable liquid and vapor
Harmful if swallowed
May be fatal if swallowed and enters airways

Precautionary Statements
Prevention
Do not eat, drink or smoke when using this product
Wash hands and face thoroughly after handling
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting/equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Wear protective gloves/protective clothing/eye protection/face protection
Skin
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
Ingestion
Rinse mouth
Do NOT induce vomiting
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
Fire
In case of fire: Use CO2, dry chemical, or foam for extinction
Explosion risk in case of fire
Fight fire with normal precautions from a reasonable distance
Evacuate area
Storage
Store locked up
Store in a well-ventilated place. Keep cool
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
None identified

3. Composition / information on ingredients

Component	CAS-No	Weight %
trans-Hex-3-ene	13269-52-8	98

4. First-aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Obtain medical attention.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Obtain medical attention.

Inhalation Remove from exposure, lie down. Move to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth resuscitation if victim ingested or inhaled the substance; induce artificial respiration with a respiratory medical device. Obtain medical attention.

Ingestion Do not induce vomiting. Obtain medical attention.

Most important symptoms/effects Breathing difficulties. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray. Carbon dioxide (CO_2). Dry chemical. chemical foam.

Unsuitable Extinguishing Media No information available

Flash Point	-12 °C / 10.4 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical
Flammable.

Hazardous Combustion Products
Carbon monoxide (CO) Carbon dioxide (CO_2)
Protective Equipment and Precautions for Firefighters
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
3	3	0	N/A

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment.
Environmental Precautions See Section 12 for additional ecological information.

Methods for Containment and Clean Up Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling Wear personal protective equipment. Ensure adequate ventilation. Avoid contact with skin and eyes. Do not breathe dust. Do not breathe vapors or spray mist. Use explosion-proof equipment. Use only non-sparking tools.

Storage Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat and sources of ignition. Flammables area.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use spark-proof tools and explosion-proof equipment.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if

	exposure limits are exceeded or if irritation or other symptoms are experienced.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	Odorless
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-113 °C / -171.4 °F
Boiling Point/Range	67 °C / 152.6 °F @ 760 mmHg
Flash Point	-12 °C / 10.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	2.90
Relative Density	0.677
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C6 H12
Molecular Weight	84.16

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable.
Conditions to Avoid	Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.
Incompatible Materials	Acids, Bases
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO_2)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information	No acute toxicity information is available for this product
Component Information	
Toxicologically Synergistic Products	No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
trans-Hex-3-ene	13269-52-8	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting
Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity
Do not empty into drains.

Persistence and Degradability No information available
Bioaccumulation/ Accumulation No information available.

Mobility No information available.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT
UN-No UN3295
Proper Shipping Name HYDROCARBONS, LIQUID, N.O.S.
Proper technical name (TRANS-3-HEXENE)
Hazard Class 3
Packing Group II

TDG
UN-No UN3295
Proper Shipping Name HYDROCARBONS, LIQUID, N.O.S.
Hazard Class 3
Packing Group II

IATA
UN-No UN3295
Proper Shipping Name HYDROCARBONS, LIQUID, N.O.S.
Hazard Class 3
Packing Group II

IMDG/IMO
UN-No UN3295
Proper Shipping Name HYDROCARBONS, LIQUID, N.O.S.
Hazard Class 3
Packing Group II

15. Regulatory information

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
trans-Hex-3-ene	-	-	-	236-261-4	-		-	X	-	-	X

Legend:
X - Listed
E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.
F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.
N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.
P - Indicates a commenced PMN substance
R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.
S - Indicates a substance that is identified in a proposed or final Significant New Use Rule
T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.
XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B).
Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.
Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b) Not applicable

SARA 313 Not applicable

SARA 311/312 Hazardous Categorization

Acute Health Hazard	Yes
Chronic Health Hazard	No
Fire Hazard	Yes
Sudden Release of Pressure Hazard	No
Reactive Hazard	No

Clean Water Act Not applicable

Clean Air Act Not applicable

OSHA Occupational Safety and Health Administration
Not applicable

CERCLA
Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals

State Right-to-Know Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security
This product does not contain any DHS chemicals.

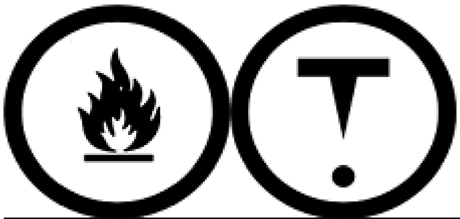
Other International Regulations

Mexico - Grade No information available

Canada

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all the information required by the CPR

WHMIS Hazard Class	B2 Flammable liquid D2B Toxic materials



16. Other information

Prepared By	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
Creation Date	27-Sep-2014
Revision Date	27-Jan-2015
Print Date	27-Jan-2015
Revision Summary	This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS)

Disclaimer

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

End of SDS

Health	2
Fire	2
Reactivity	0
Personal Protection	J

Material Safety Data Sheet
N-Methyl-2-pyrrolidinone MSDS

Section 1: Chemical Product and Company Identification

Product Name: N-Methyl-2-pyrrolidinone

Catalog Codes: SLM2023, SLM3397

CAS#: 872-50-4

RTECS: UY5790000

TSCA: TSCA 8(b) inventory: N-Methyl-2-pyrrolidinone

CI#: Not available.

Synonym: N-Methyl Pyrrolidone

Chemical Name: N-Methyl-2-Pyrrolidinone

Chemical Formula: C5H9NO

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
{N-}Methyl{-2-}pyrrolidinone	872-50-4	100

Toxicological Data on Ingredients: N-Methyl-2-pyrrolidinone: ORAL (LD50): Acute: 3914 mg/kg [Rat]. 5130 mg/kg [Mouse]. DERMAL (LD50): Acute: 8000 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, kidneys, lymphatic system, Urinary system, bone marrow. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.

Skin Contact: Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops.

Serious Skin Contact: Not available.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation: Not available.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Combustible.

Auto-Ignition Temperature: 346.11°C (655°F)

Flash Points: CLOSED CUP: 92.778°C (199°F). OPEN CUP: 95.556°C (204°F).

Flammable Limits: LOWER: 1.3% UPPER: 9.5%

Products of Combustion: These products are carbon oxides (CO, CO2), nitrogen oxides (NO, NO2...).

Fire Hazards in Presence of Various Substances:
Slightly flammable to flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Combustible material. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of

insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as oxidizing agents, reducing agents, acids, alkalis.

Storage:
Hygroscopic. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Do not store above 24°C (75.2°F). Preferably refrigerate.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection: Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 25 STEL: 75 (ppm) [United Kingdom (UK)] TWA: 103 STEL: 309 (mg/m3) [United Kingdom (UK)] TWA: 10 from AIHA TWA: 40 (mg/m3) from AIHA Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Amine like.

Taste: Not available.

Molecular Weight: 99.14 g/mole

Color: Colorless to light yellow.

pH (1% soln/water): Not available.

Boiling Point: 202°C (395.6°F)

Melting Point: -24°C (-11.2°F)

Critical Temperature: 451°C (843.8°F)

Specific Gravity: 1.026 (Water = 1)

Vapor Pressure: 0 kPa (@ 20°C)

Vapor Density: 3.4 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -0.5

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility:
Miscible with Castor Oil. Miscible with water, lower alcohols, ketones, ethyl acetate, chloroform and benzene. Moderately soluble in aliphatic hydrocarbons and dissolves many organic and inorganic compounds.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excess heat, moisture, incompatibles

Incompatibility with various substances:
Reactive with oxidizing agents, reducing agents, acids, alkalis. Slightly reactive to reactive with moisture.

Corrosivity: Not available.

Special Remarks on Reactivity:
Hygroscopic. Incompatible with reducing agents, strong alkalies, strong mineral acids. Reacts with chlorinating agents (e.g. cobalt chloride, thionyl chloride, phosphorous oxychloride, pentachlorophosphorous to form the amide. Reacts with sulfur and carbon disulfide at high temperatures and pressures.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Eye contact. Inhalation.

Toxicity to Animals:
Acute oral toxicity (LD50): 3914 mg/kg [Rat]. Acute dermal toxicity (LD50): 8000 mg/kg [Rabbit].

Chronic Effects on Humans:
MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. May cause damage to the following organs: blood, kidneys, lymphatic system, Urinary system, bone marrow.

Other Toxic Effects on Humans:
Hazardous in case of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (maternal effects - post implantation mortality, fetotoxicity) and birth defects based on animal. May affect genetic material. May cause cancer (tumorigenic) based on animal data.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. May be absorbed through skin. Eyes: Causes moderate eye irritation. Inhalation: Causes respiratory tract irritation. May affect respiration (dyspnea), gastrointestinal tract (abdominal pain, nausea, voiting and inflammation of gums and mouth, behavior/Central Nervous system (somnolence, muscel weakness, dizziness, drowsiness, headache), and urinary system. Ingestion: May cause gastrointestinal tract irritation with nausea, vomiting and diarrhea. May affect behavior/Central Nervous System (similar symptoms to inhalation) metabolism, blood and urinary tract.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).

Identification: Not applicable.

Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: N-Methyl-2-pyrrolidinone Minnesota: N-Methyl-2-pyrrolidinone Massachusetts RTK: N-Methyl-2-pyrrolidinone New Jersey: N-Methyl-2-pyrrolidinone New Jersey spill list: N-Methyl-2-pyrrolidinone TSCA 8(b) inventory: N-Methyl-2-pyrrolidinone TSCA 4(a) final test rules: N-Methyl-2-pyrrolidinone TSCA 8(a) IUR: N-Methyl-2-pyrrolidinone TSCA 12(b) one time export: N-Methyl-2-pyrrolidinone SARA 313 toxic chemical notification and release reporting: N-Methyl-2-pyrrolidinone

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F).

DSCL (EEC):
R36- Irritating to eyes. S2- Keep out of the reach of children. S46- If swallowed, seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 2

Reactivity: 0

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:
Not applicable. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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